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A workflow for the sustainable development of closure models for bubbly flows

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Abstract

Many years of research in developing closure models for polydisperse bubbly flows have produced a plethora of empirical and semi-empirical models. The continuous development and analysis of such models requires their constant validation with the steadily increasing number of validation cases in the literature.

In this paper we present a pipeline for the fully-automated analysis of OpenFOAM simulations using the Snakemake workflow management system. The pipeline is applied to an extensive collection of well-established validation cases for bubbly flows and allows the fast and efficient production of large amounts of results that are summarized in well-structured reports. An optional post-processing step introduces a fuzzy logic controller developed for the detailed analysis of these results by quantifying the agreement of the simulation with the available experimental data. It is demonstrated how such quantification enables the systematic evaluation of new closure models and contributes to a more sustainable model development.

Keywords:

Baseline, bubbly flow, OpenFOAM, workflow, artificial intelligence

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1 1. Introduction

Understanding and predicting multiphase flows is crucial for the devel-2 opment of reliable, safe and efficient devices in the nuclear, chemical, energy 3 and oil-and-gas industry. Computational fluid dynamics (CFD) has proven 4 to be an indispensable tool that adds to a better understanding of multiphase 5 flows on all relevant scales, from single bubbles to the flow in large industrial 6 components. Much effort was focused on achieving predictive capabilities 7 of CFD simulations during the last decades. Today, the Eulerian-Eulerian 8 two-fluid methodology is widely used for analysing multiphase flows on the 9 industrial component-scale. Low computational cost and great flexibility in 10 terms of possible flow geometries have made it the state-of-the-art approach 11 for multiphase flow analysis in the industry. The reliability of results depends 12 on the availability of accurate closure models and their correct application. 13 Although good predictions can often be obtained for single cases, there is an 14 ongoing effort to reduce the empiricism of models in favour of more mecha-15 nistic formulations for a better accuracy and generality of these models. 16

Decades of developing new models for Eulerian-Eulerian CFD have pro-17 duced a vast amount of literature on the subject, and a huge number of 18 both models and validation cases [1, 2, 3]. For each required Euler-Euler 19 closure a multitude of empirical or semi-empirical models exists in the lit-20 erature from which the CFD engineer is free to choose. This accumulation 21 of models makes it increasingly difficult to give best practice guidelines for 22 the simulation of bubbly flows. Evaluating new models and comparing them 23 against the plethora of available alternatives becomes an increasingly tedious 24 endeavour. 25

However, the huge amount of data to be found in the literature offers the 26 opportunity to apply workflow tools for a faster and more efficient process-27 ing of CFD data. In other fields of research, such as bio-informatics [4] and 28 RNA sequencing in particular [5], the development of workflows has already 29 proven to be fundamental for gaining a deeper understanding of large data 30 sets. The enormous amount of CFD data produced from existing validation 31 cases and the increasing number of closure models make a fast and efficient 32 tool to process all this data a crucial part of the Euler-Euler model devel-33 opment in the future. Furthermore, such automation allows us to explore 34 the possibility of including data science and artificial intelligence tools in the 35 analysis and evaluation process of new Euler-Euler models. 36

37

In Section 2 of this paper we describe the current status of Eulerian-38 Eulerian CFD modeling of multiphase flows. We will review the conven-39 tional way of developing and testing new models and highlight the issues 40 that arise from following such an approach. We then present the alternative 41 'baseline' strategy [6] developed at Helmholtz-Zentrum Dresden-Rossendorf 42 (HZDR), which aims at converging towards a fixed set of universal closure 43 models, so-called baseline models. An overview of the current collection of 44 validation cases for baseline model testing available at HZDR is given. In 45 Section 3 we then present the Snakemake workflow, which was developed 46 for the fully-automated pre-processing, running and post-processing of the 47 extensive amount of OpenFOAM cases in our collection. Section 4 will apply 48 fuzzy logic, a subset of artificial intelligence, for the evaluation of simulation 49 results. We will describe the parts of a fuzzy logic controller, designed to 50 infer from two error metrics an output metric that allows us to compare the 51 performance of new Euler-Euler models with the baseline model set. Results 52 of a demonstration case are then presented in Section 5 where we test a new 53 lift force correlation against the current baseline model. We describe the per-54 formance of the workflow and present validation graphs of selected cases to 55 demonstrate the fuzzy logic evaluation. An overview of fuzzy logic results for 56 the entire case collection aims to demonstrate the potential of such artificial 57 intelligence tools for a sustainable Euler-Euler model development. Conclu-58 sions and an outlook to where our future work is going is given in Section 50 6. 60

61 2. Background

62 2.1. Conventional Euler-Euler model development

The description of two-phase flows with the Eulerian-Eulerian methodol-63 ogy requires many closure models. Closure models need to describe all the 64 detailed flow phenomena, which the usually coarse computational grid can-65 not resolve. For polydisperse bubbly flows a dozen such closures is needed: 66 interfacial force closures, i.e. drag, shear lift, turbulent dispersion, virtual 67 mass and wall lubrication forces [7], turbulence closures for the shear and 68 bubble-induced turbulence of the liquid phase [8], and closures describing 60 the polydispersity of bubbles, i.e. a population balance model, and models 70 for both coalescence and breakup events [9]. A lot of different model options 71 for each of these closures have emerged in the literature, each of which comes 72 with a multitude of adjustable model parameters. 73

Table 1 lists a selection of such models suitable for the modeling of bubbly 74 flows, part of which are provided by OpenFOAM [10] and by the HZDR 75 Multiphase Addon for OpenFOAM [11]. Listed are five drag models, three lift 76 models, three models for turbulent dispersion, two for vitual mass and four 77 for wall lubrication, three different turbulence models for the liquid and three 78 different models for bubble-induced turbulence, two different approaches for 79 population balance modeling, five different coalescence and four different 80 binary breakup models. These 34 options alone give a total of 129600 possible 81 model combinations. This number becomes even more extensive considering 82 all the models in the literature not vet included in the HZDR model library. 83 Numerous model parameters inherent in every sub-model further add to the 84 complexity. The description of polydisperse bubbly flows using the Euler-85 Euler approach is inarguably based on a highly complex set of intricately-86 linked models making the interpretation of CFD results extremely difficult. 87

Table 1: Closure models for polydisperse bubbly flow available with the HZDR Multiphase Addon for OpenFOAM [11]. The current baseline model set is indicated in bold text.

Required closures		Model options	Parameter
Interfacial	Drag	Ishii and Zuber [12]	-
forces		Schiller and Naumann [13]	-
		Tomiyama et al. [14]	-
		Tomiyama et al. [15]	-
		Tomiyama et al. [16]	-
	Shear lift	Tomiyama et al. [17]	-
		Legendre and Magnaudet [18]	-
		Moraga et al. [19]	-
	Turbulent	Burns et al. [20]	1
	dispersion	Gosman et al. [21]	1
		Lopez de Bertodano [22]	1
	Virtual	Crowe et al. [23]	1
	mass	Lamb [24]	-
	Wall	Hosokawa et al. [25]	-
	lubrication	Antal et al. [26]	2
		Frank [27]	3
		Tomiyama [28]	1
Turbulence	Shear-	k-omega-SST [29]	12
	induced	k-epsilon [30]	6
		k-omega [31]	5
	Bubble-	Ma et al. [32]	-
	induced	Rzehak and Krepper [33]	-
		Sato and Sadatomi [34]	1
Poly-	Population	Class method [35]	-
dispersity	balance	Ishii et al. [36]	-
	Coalescence	Liao et al. [9]	9
		Coulaloglou and Tavlarides [37]	2
		Lehr et al. [38]	2
		Luo [39]	2
		Prince and Blanch [40]	3
	Breakup	Liao et al. [9]	4
		Lehr et al. $[38]$	-
		Laakkonen et al. [41]	4
		Luo and Svendsen [42]	3

There is no consensus about the use of any of those closure models. In the literature usually a different set of models is chosen by each research group [43, 1, 7, 44]. Model constants tend to be tuned for each specific validation case. Despite a large number of publications on the model development for the last two decades little progress is seen towards Eulerian-Eulerian simulations with reliable predictive abilities [6].

94 2.2. The 'Baseline' Strategy

The aim of the baseline strategy at HZDR is to arrive at a single univer-95 sal set of Eulerian-Eulerian two-fluid models that can predict bubbly flows 96 in any flow configuration. Baseline models should offer a certain range of 97 applicability regarding the local flow characteristics. The baseline model set 98 is fixed, as are the model constants. For different flow situations the contri-99 bution of each of the phenomena listed in Table 1 will of course vary, but the 100 baseline model set should predict such changes without any further tuning. 101 As described by Lucas et al. [6] for the sake of generality the models chosen 102 for each phenomena should preferably be mechanistic models that are based 103 on local flow conditions rather than empirical models derived from observa-104 tions made in a specific experiment. The baseline model set should produce 105 convincing results for a large range of different validation cases in order to 106 prove its predictive abilities for future cases. 107

Table 1 lists the current set of baseline models for polydisperse bubbly flow at HZDR in bold letters. Find the detailed equations for these models in Liao et al. [8]. Over the years the models listed here have proven to repeatedly produce good results for a variety of cases [9, 7, 8].

Figure 1 illustrates the general process of updating this fixed set of base-112 line models in case a new model has been developed or found in the literature. 113 In a first step the new model needs to be analysed regarding the model re-114 quirements of the baseline model set. Various features need to be checked, 115 such as a physical and mechanistic basis of the model, its generality or its 116 derivation from advanced experiments. If the advantages of the new model 117 become apparent, it will then be tested in a next step. This part of the 118 process is essential as it aims to demonstrate an overall improvement of the 119 CFD predictions for a collection of cases. This case collection contains an 120 extensive selection of validation cases, which will be described in the next 121 section. Generally, a new model will replace the current baseline model if an 122 improvement for the majority of our validation cases can be demonstrated. 123

¹²⁴ During the continuous model development we try to identify deficiencies of ¹²⁵ models, in which we should invest our efforts for further improvement.

As illustrated on the right hand side of the flow diagram in Figure 1 a 126 model update can be considered even if overall case results do not improve. 127 The advantages of a new model then need to outweigh the deterioration of 128 results. The coupling of physical phenomena is complex making a straight-129 forward model evaluation impossible at times. Worse results obtained with 130 a better model can be caused by the interdependence of the current set of 131 baseline models, where potential shortcomings of one model are possibly 132 compensated by the tuning of another. 133



^{*}Performance= agreement with experiments/DNS and numerical stability/computing time



¹³⁴ 2.3. The current collection of cases at HZDR

As described above, the process of testing new models involves the simulation of a large number of validation cases. The case collection at HZDR currently contains 56 pipe and bubble column cases, with the case number continuously growing. Cases differ regarding their geometry, gas injection, bubble sizes, water quality etc. Keywords were introduced to categorise the

cases and their sub-cases as illustrated in Table 2. The keywords illustrated 140 are not complete, but rather form a starting point to label existing cases. 141 More cases are to be added in the future in order to diversify the collection 142 and its keywords, as well as to simply increase the amount of validation data. 143 Case setups are standardised using the best-practice guidelines given in 144 Lucas et al. [45] and simulated using the HZDR Multiphase Addon for Open-145 FOAM, which was customized and extended for the various model develop-146 ments at HZDR. All cases are under Git version control and managed in 147 GitLab [46]. GitLab Continuous Integration and Continuous Development 148 (CI/CD) mechanisms allow an efficient maintenance of the case collection, 149 as well as its extension by new cases. 150

Cases		Geo met	ry	Gas jecti	in- on	Gas pha	Gas Bubble size change		Bubble Water quality sizes			State		Devel- opment					
		Pipe	Bubble column	Bottom	Wall	one-gas	multiple-gas	Fixed	Density-change	Coalescence-breakup	Monodisperse	Polydisperse	Filtered	Tap water	Contaminated	Steady-state	Transient	Fully developed	Developing
Wang et al.	W1	Х		х		х		х			х		х			х		Х	
(1987)	W2	X		X		X		X V			X		X			X		X	
Liu and Bankoff	LB1	Ŷ		x		Ŷ		x			x		x			x		x	
(1993)	LB2	X		X		X		x			X		x			X		X	
Liu (1998)	L11A	Х		х		х		х			х			X		Х		Х	
	L21B	X		X		X		X			X			X		X		X	
	L21C	X		X		×		Н¥-			X			X		X		X	
Pfleger (1999)		Ê	x	x		<u> </u>	x	<u> </u>		x	<u> </u>	x		x		<u>^</u>	x		x
Deen (2001)			X	X		х	<u> </u>	x			х				х		X		X
Hibiki (2001)	H11	Х		Х		Х		Х			Х		х			Х		Х	
	H12	X		X		X		X			X		X			X		X	
	H13	X		X		×		Н¥-			X		×			X		X	
	H32	Ŷ		Ŷ		Î		Î			Ŷ		Î			Ŷ		Ŷ	
	H33	X		X		X		x			X		x			X		X	
Shawkat (2008)	S21	Х		Х		Х		Х			Х		Х			Х		Х	
	S23	X		X		X		X			X		X			X		X	
	S31 622	X		X		×		Н Х			X		X			X		X	
Hosokawa	H11	x		x		x		Î			x		Ê	x		x		x	
(2009)	H12	X		X		X		X			X			X		X		X	
	H21	X		X		X		X			X			X		X		X	
Alden et al	H22	X	v	X		×		×		<u> </u>	X	-		X		X	v	X	v
(2012)	3		X	x		x	×	x			x	X		X			X		X
Hosokawa and	H1	х		X		x		x			x			X		х	<u> </u>	х	~
Tomiyama	H2	Х		Х		Х		Х			Х			X		Х		Х	
(2013)	H3	X		X		X		X			X			X		X		X	
Kim (2016)	H4	×		÷		÷		₩÷-			÷			×		÷		×	
Kiiii (2016)	K1 K2	Ŷ		Ŷ		Î		Î			Â			Ŷ		Ŷ		Ŷ	
	K3	X		X		X		X			X			X		X		X	
	K4	Х		Х		Х		х			Х			X		Х		Х	
Lucas et al.	fd_19	X		X		X		ТХ Х				X	X			X		X	
(2005)	fd 39	Ŷ		Ŷ		Î		Î				x	Î			Ŷ		x	
	fd_41	X		X		X		X				X	X			X		X	
	fd_59	X		X		X		X				X	X			X		X	
	fd_61	X		X		X		Н¥-				X	× ×			X		X	
	fd 85	Ŷ		Ŷ		Î		Ê				x	Î			Ŷ		Ŷ	
	d_19	X		X		X			X	X		X	X			X			X
	d_37	X		X		X			X	X		X	X			X			X
	d_39	X		X		X			X	X		X	 ×			X			X
	d 59	x		Ŷ		x			x	X		X	Ŷ			x			Ŷ
	d_61	X		X		X			X	X		X	X			X			X
	d_63	X		X		X			X	X		X	X			X			X
	d_85	X		X	v	×			X	X		X	ا ب			X			X
(2010)	40	Ŷ			x	x			-	X		X	Î x	-		Ŷ			Ŷ
、·=·-/	41	X			X	X				X		X	X			x			X
	42	X			X	X				X		X	X			X			X
	52	X			X	IX I			1	∣X		X	ιX	1		X			X

Table 2: Overview of cases with all active keywords.

¹⁵¹ 2.4. The challenge of evaluating new models

Each case in the case collection produces results that are compared to validation data, i.e. experimental data. Some fully-developed cases produce steady-state results, for other transient cases the results need to be timeaveraged. Typical graphs for analyzing results are gas void fraction profiles, liquid and gas velocity profiles, sometimes profiles of turbulent quantities, such as the turbulent kinetic energy. Transient cases produce the respective mean values of the same quantities.

In case a new model is tested the computed results additionally need to be compared with the old baseline reference solution. For each of the plots various curves need to be compared: the computed result using the new model, the reference result obtained with the current baseline model set and the measured data for validation. Examples of such graphs are given in Figure 2. The reason why this kind of evaluation is a time-consuming challenge is twofold:

First, the sheer number of results to evaluate is extensive and hard to 166 handle. It is difficult to demonstrate an overall improvement for the total 167 number of currently 56 cases, each of which produces three to five graphs. 168 Assuming only three graphs for each case, a total of 168 plots has to be 169 evaluated. These plots are typically scattered across case folders. The issue 170 becomes even more pressing with an increasing number of cases and plots, 171 which for baseline development purposes is intended. Therefore, a **workflow** 172 for an automated production of such graphs and their neat presentation in a 173 single report is developed, as will be presented in Section 3. 174

Second, the information in some graphs can be vague and the decision if there is an improvement of results can become rather subjective. Plotted results need to be evaluated and compared, which is typically done during long and difficult discussions among experts. For a better qualitative judgement and quantification of the performance of new models we will therefore introduce a **fuzzy logic approach** in Section 4 that is meant to aid the decision-making process.

182 3. Automation of cases in a workflow

Workflow engines are designed to automate the successive execution of commands and applications for large-scale data analyses. The generation of data via workflows follows so-called FAIR principles [47] for a good management of scientific data, which should be transparent and reproducible. Out of a large number of potential workflow systems (such as [48] etc.) for the work presented here we chose Snakemake and developed a workflow, which will be described in the next sections.

190 3.1. The Snakemake library

Snakemake is a general purpose Python library originally developed for
 applications in the field of bio-informatics [4]. The library allows to build
 complex algorithms that process large data-sets using scientific software, and
 manages the resulting output.

As described by Evdokimov et al. [49] the Snakemake library provides several features that make it a suitable framework for managing the extensive amount of CFD simulations we are interested in here, and their subsequent analysis:

- The syntax of Snakemake offers great flexibility in terms of the scripting
 languages that jobs can be composed of, which allows individual case by-case setups.
- The library comes with interfaces to common cluster schedulers required for high-performance computing.
- Snakemake was built for parallization enabling us to spawn parallel case
 jobs on separate nodes of a cluster to maximize speed. Furthermore,
 it can adapt the number of jobs in execution to the allocated workflow
 resources.
- Its modularity allows to rerun downstream analysis and re-process subsets of jobs without the need to rerun the entire pipeline.
- The post-processing output is aggregated and put into a single place with the possibility to include results of hundreds of cases.
- On the low-level a case-by-case approach allows to easily split work among researchers in a team, and

• On the top-level common CI/CD software design practices are applicable and allow the consistent integration of the library into our existing case repository.

217 3.2. Workflow overview

The details of the workflow on both the case- and the top-level, are described and illustrated in Evdokimov et al. [49]. The following section will briefly summarize the main steps and workflow specifications relevant for our baseline model development.

The workflow consists of the following three steps reflecting a *bottom-up* method of determining job execution:

1. During a *configuration step* an algorithm searches in sub-folders for 224 Snakefiles that define the specifications of the pre-processing, solv-225 ing and post-processing job for each individual case. Snakefiles are 226 designed in such a way that they allow the independent workflow ex-227 ecution of a selection of cases. Larger cases that inlude extensive 228 parameter-variations (e.g. Lucas et al. [50] with hundreds of systematic 229 case setup variations) are setup via templates building file structures 230 and sub-cases. Once the *configuration* step has completed, the estab-231 lished file structure is ready for launching the workflow. 232

233
 2. The workflow then runs the selected cases during the *solution* step.
 Workflow reports containing the plots of all the cases are produced
 using the report-generating feature embedded in the Snakemake library.

3. A third optional *post-processing* step produces a case-by-case overview
of the agreement of the computed results with the validation data. This
step is particularly important for the testing of new baseline models and
incorporates the fuzzy logic system described in Section 4. Computed
results are not only compared to the validation data, but also to the
reference solution obtained by applying the baseline model set.

242 3.3. Workflow reports

Snakemake reports are generated in the form of static web-pages, which are easily deployed and shared on a web-server. CI/CD mechanisms for the workflow execution allow deploying reports onto web-servers as soon as a certain job has finished making results instantly accessible to the whole research team. A demonstration of the final workflow report via screenshots is presented in Evdokimov et al. [49]. A side panel lists all cases simulated, which upon selection will show the corresponding validation plots on the main page for inspection. For further illustration purposes we refer to the demonstration report provided by the Snakemake library on a public webpage [51]. This report gives an impression of the typical report structure for results.

The Snakemake workflow gives us an efficient tool to produce a large amount of plots and to represent them in a well-structured report. The evaluation of these reports for the baseline model development remains the task of the user, but can be supported by artificial intelligence tools, such as the fuzzy logic controller described in the next section.

4. Evaluation of results

The decision whether or not a computed *simulation* result is better than the *baseline* reference solution can be quite easy to make, such as in the plot illustrated on the left hand side of Figure 2, or it can be less obvious, such as the example on the right hand side.



Figure 2: Gas void fraction profiles of fullyDeveloped_39 (left) and case L11A (right).

Fuzzy logic is a subset of artificial intelligence, which can accommodate the imprecision of the real world and support such a decision-making process. By using linguistic variables fuzzy logic can deal with imprecise, vague and uncertain information and approximate human reasoning.

The scikit-fuzzy library ([52], [53]) allows the integration of such fuzzy 268 logic tools into our workflow, where it can be utilized for the testing of new 269 models. From the system design point of view the library takes responsibility 270 for the correct and robust implementation of the underlying algebra and the 271 numerical algorithms, while on the top level we investigate metrics and their 272 value boundaries suitable to our multiphase CFD problems. In essence, we 273 propose a *fuzzy logic controller* for the purpose of evaluating and comparing 274 CFD results. In the next sections we briefly describe how this controller 275 works. 276

277 4.1. The fuzzy logic system

Fuzzy logic uses a specific terminology, which is briefly introduced here for a better understanding of the following sections. When a value is referred to as being crisp this means it is explicit and concise. *Fuzzification* is the process of decomposing such crisp values into a spectrum of different

linguistic categories, referred to as fuzzy sets. A typical fuzzy logic system 282 is illustrated in Figure 3. The system consumes and *fuzzifies* several crisp 283 inputs, which means numerical floating-point or integer values are mapped 284 onto linguistic sets via membership functions. These membership functions 285 are normalized and might be considered as weight-factors of the expert sys-286 tem. Inference logic combines the numerous fuzzy input sets via a set of 287 rules to produce *fuzzy output sets*, which themselves represent linguistic sets. 288 Finally, these output sets are summed up, *defuzified* and mapped onto a 289 single crisp output value. 290



Figure 3: Schematic of a fuzzy logic system.

The inputs specified for the fuzzy system demonstrated here are two error metrics that will be described in the next section. One of the advantages of the fuzzy logic approach lies in its modularity allowing us to extend this list of fuzzy input variables in the future. In our case the desired output of the fuzzy logic system is a value between 0 and 1 quantifying how good the computed CFD result agrees with the measured validation data. We will refer to this crisp output as **goodness-value** *G* of the CFD prediction.

298 4.2. The crisp inputs: error metrics

The crisp inputs for our fuzzy logic system are specific error metrics that describe the similarity of two curves: our computed result, such as the gas void fraction profile, and the corresponding experimental data for validation. Various metrics could be used, but for demonstration purposes the number here is limited to two, which complement each other. The error metrics below are defined using the example of evaluating sorted sets of gas void fraction data. Hereby, the sorted set represents the radial profile in case of round ³⁰⁶ geometries or the lateral profile in case of rectangular columns. Metrics for³⁰⁷ the other validation fields are computed accordingly.

As a quantitative measure the **Mean relative error MRE** is defined as:

$$MRE = \frac{1}{N} \sum_{n=1}^{N} \frac{|\alpha_{n,sim} - \alpha_{n,exp}|}{\bar{\alpha}_{exp}}$$
(1)

with N being the number of values, the computed values of the gas void 310 fraction α_{sim} and the experimentally measured ones α_{exp} , and $\bar{\alpha}$ the arith-311 metic average. The MRE describes the quantitative distance between two 312 curves along the ordinate. It is normalized by the mean experimental value 313 for the entire profile in order to avoid a heavier penalty of discrepancies for 314 data points with smaller experimental values. Possible values for the MRE 315 range from 0 to ∞ . We therefore limit values to a maximum of 1. Note that 316 a case with a MRE > 1 therefore will not receive a heavier penalty than cases 317 with a MRE = 1. Most cases in our collection, however, fall into the range 318 of 0 < MRE < 1. 319

As a qualitative measure the **Pearson correlation coefficient PCC** is defined as the covariance of the two gas void fraction data sets divided by the product of their standard deviation:

$$PCC = \frac{\sum_{n=1}^{N} (\alpha_{n,sim} - \bar{\alpha}_{sim}) (\alpha_{n,exp} - \bar{\alpha}_{exp})}{\sqrt{\sum_{n=1}^{N} (\alpha_{n,sim} - \bar{\alpha}_{sim})^2} \sqrt{\sum_{n=1}^{N} (\alpha_{n,exp} - \bar{\alpha}_{exp})^2}}$$
(2)

The Pearson correlation coefficient determines the similarity of the two 323 data sets, i.e. the shapes of the two curves. The range of the Pearson 324 coefficient is -1 < PCC < 1. Examples of PCC values are illustrated in 325 Figure 4, where simulation profiles are compared with experimental data. A 326 negative coefficient indicates a negative linear correlation and a low similarity 327 between curves, such as in the case of a predicted wall peak for a measured 328 core peak profile. A positive coefficient represents a positive linear correlation 329 of the data set meaning a high similarity of shapes, as illustrated for the 330 almost matching profiles on the right hand side. 331



Figure 4: Pearson correlation coefficients computed for different data sets of gas void fraction profiles.

The PCC criteria is not sensitive to shifts of the profiles along the ordinate, but sensitive to shifts along the abscissa. Thus, it complements the MRE metric, which is mainly sensitive to shifts along the ordinate.

335 4.3. Membership functions

A fuzzy set of linguistic terms is assigned to each input and output metric as illustrated in Table 3. The process of turning crisp variables into linguistic sets is termed *fuzzification*.

Variable	Linguistic sets	Parameters a,b,c
MRE	"low"	0, 0, 0.3
	"medium"	0,0.3,1.0
	"high"	0.3, 1.0, 1.0
PCC	"high"	0.4, 1.0, 1.0
	"medium"	-1.0, 0.4, 1.0
	"low"	-1.0, -1.0, 0.4
G	"perfect"	0.7, 1.0, 1.0
	"good"	0.5,0.7,0.9
	"tolerable"	0.3,0.5,0.7
	"bad"	0.1,0.3,0.5
	"defect"	0.0, 0.0, 0.3

Table 3: Linguistic sets assigned to each variable.

Membership functions $\mu_i(x)$ tie the input and output variables x for each linguistic set item i of the above table to a number, which can be understood as an impact value. Piece-wise *triangle* functions are used:

$$\mu_{i}(x) = \begin{cases} 0 & x \le a \\ \frac{x-a}{b-a} & a \le x \le b \\ \frac{c-x}{c-b} & b \le x \le c \\ 0 & c \le x \end{cases}$$
(3)

with parameters a, b and c specified separately for each item of the set as listed in Table 3. The triangle-shaped membership functions assigned to the linguistic terms listed in Table 3 are illustrated in Figure 5.



Figure 5: Membership functions for the fuzzy input and output sets. The x axis represents the crisp value space, the y value represents the membership function output value for each linguistic term.

For a specific metric value the membership function output represents a fuzzy degree of membership in the qualifying linguistic set. Thus, value intervals are constrained to a uniform range from zero to one for all input and output metrics, and the fuzzy set is *normalized*. For a crisp value x a fuzzy set now is defined as a pair:

$$A(x) = (i, \mu_i(x)) \tag{4}$$

where item *i* is a linguistic term and $\mu_i(x)$ the membership function expressing the degree of membership in that term.

352 4.4. Fuzzy rule base

Operations can be defined on the various fuzzy sets by means of their membership function. This allows us to prescribe an intuitive rule base, which is easy to interpret.

The current workflow evaluation consists of the following five rules:

- $_{357}$ 1. If PCC:low AND MRE:high ightarrow Defect G
- 2. If (PCC:low AND MRE:medium) OR (PCC:medium AND MRE:high) \rightarrow Bad G
- 360 3. If (PCC:medium AND MRE:medium)
- OR (PCC:high AND MRE:high)
- $_{
 m 362}$ OR (PCC:low AND MRE:low) ightarrow Tolerable G
- 4. If (PCC:high AND MRE:medium) OR (PCC:medium AND MRE:low) \rightarrow Good G
- $_{365}$ 5. If PCC:high AND MRE:low \rightarrow Perfect G

A simplified visual representation for the target "Goodness" metric G is illustrated in Figure 6.



Figure 6: A schematic view of the relationship between the fuzzy input metrics and the output metric G.

Fuzzy operators are applied to obtain one value representing the result of each rule. Logical *min/max* operators correspond to the AND/OR rules mentioned above [54]. Input for these operators are the membership values of the fuzzified input variables, and the output is a single value.

An example is illustrated in Figure 7 for a case with PCC = 0.49 and MRE = 0.36. A single fuzzy rule, rule 4 for the fuzzy set *Good* of the G metric, is exemplified. The condition (PCC:high AND MRE:medium) OR (PCC:medium AND MRE:low) can be translated into max(min(0.15, 0.91), min(0.85, 0)) = 0.15. This output is used for the implication of the fuzzy rule as described in the next section.



Figure 7: Application of rule 4 via fuzzy operators for an example of two input metrics.

378 4.5. Implication and defuzzification

An implication method turns the single output value into the consequence of the fuzzy rule. The consequent fuzzy sets are represented by the membership functions of the output sets. Input for the implication method is the value outputs given by each of the antecedent rules, such as rule 4 above.

Mamdani-type inference was applied for the implication process as it is an 383 intuitive method, well-suited to human input, allowing an interpretable rule 384 base and with widespread acceptance [54]. It works with the *min* implication 385 operator to infer the output functions, as it is illustrated for rule 4 on the right 386 hand side of Figure 7. The five fuzzy rules produce the output functions for 387 the five potential sets of the goodness variable. Figure 8 illustrates the whole 388 inference process for the above example with PCC = 0.49 and MRE = 0.36. 389 In the example only three out of five output sets qualify during the inference 390 step. 391



Figure 8: Inference system including all rules for an example of two input metrics.

The consequent functions of all rules then need to be aggregated, which 392 is done by a simple max function. In a last step the aggregated function is 393 defuzzified. The scikit-fuzzy library allows to choose from several meth-394 ods suggesting different trade-offs between the smoothness of the response 395 surface and the robustness of the final defuzzification step. In the model 396 evaluation attempted here we tried to track the smallest variations to allow 397 a continuous differentiation of results. Therefore, our chosen defuzzification 398 method relies on area measurements of the aggregated result. Defuzzification 399 is performed by the *bisector* method, which finds the vertical line that di-400 vides the aggregated result into two sub-regions of equal area. The response 401 surface of our current two-input, one-output, five-rule fuzzy logic system is 402 illustrated in Figure 9. 403



Figure 9: Response surface of the fuzzy logic system.

404 4.6. Evaluation for the case collection

The fuzzy logic approach offers a convenient framework for an evaluation 405 algorithm, which could be easily repurposed, extended and redefined. The 406 alternative usage of an equivalent multidimensional target function requires 407 the strict definition of potentially controversial input values fitting a specific 408 output metric. Fuzzy logic makes it easy to reach a consensus amongst re-409 searchers by using relations between linguistic sets derived from these values. 410 Errors divided into a low, medium and high subset are easily agreed on, but 411 certain values fitting these sets are not. 412

As described above for each case in the case collection several fields are investigated for the validation of the CFD results, e.g. gas void fractions or velocity profiles. A goodness value G is computed for each of those individual validation fields and is meant to describe how good the predicted profile agrees with the experimental data. The average over all these individual goodness values for the available validation fields produces a single value for each case. This single value represents the overall goodness of the CFD prediction for the case investigated. In the future different weightings for the various validation fields could be considered.

When testing a new model the above procedure is done twice, for the results using the new model and for the reference solution obtained with the baseline model set. An improvement or deterioration of the CFD results for a specific case can then be expressed via the difference in the overall goodness of the computed and the baseline result.

428 5. Demonstration case: Testing a new lift force correlation

To demonstrate the efficiency of the baseline workflow and its fuzzy logic 429 tool, this section will now investigate results when testing a new lift force 430 correlation. We will refer to the results obtained with the Tomiyama correla-431 tion [17] as *baseline* results, and the results with a new correlation for the lift 432 coefficient proposed by Hessenkemper et al. [55] as *computed* results. This 433 section does not aim to validate the new correlation, but to demonstrate the 434 benefits and future potential of the developed workflow tools in assisting the 435 baseline model development. 436

We will give an impression of the performance and reporting features of the workflow when analysing a certain selection of cases. The evaluation of results via fuzzy logic will then be verified for a selected case. Finally, an overview of the overall goodness evaluation for all cases is presented.

441 5.1. Workflow performance

For the following analysis we restrict our selection of respository cases to the ones that have already been published elsewhere, as listed in Table 4. The individual case setups in OpenFOAM are described in the references given, and are to be found in the *HZDR Multiphase Case Collection for OpenFOAM* [56]. Including all sub-cases the total number of cases investigated here is 36. The simulation of each individual sub-case demands three to eight processors and an execution time of up to two hours.

Experimental reference	Cases	Setup	CPUs/Case
Hosokawa and Tomiyama [57]	4	[58]	4
Liu [59]	4	[58], [60]	4
Shawkat et al. [61]	4	[60]	4
Hosokawa and Tomiyama [62]	4	[60], [63]	8
Kim et al. [64]	4	[63]	8
Lucas et al. [50]	16	[65]	3

Table 4: List of cases for the workflow demonstration.

The Snakemake workflow processes all these cases with a total execution time of \sim 5h (the entire case collection takes \sim 10h). A total of 236 plots (baseline relevant and auxiliary) is generated automatically. In the plots relevant for the baseline evaluation the computed results are compared to ⁴⁵³ both the experimental data and the reference solution. Examples of such
⁴⁵⁴ plots are illustrated in Figure 2. The fuzzy logic evaluation of these results
⁴⁵⁵ during the optional post-processing step is done with an execution time of
⁴⁵⁶ only four minutes.

457 5.2. Verification of the fuzzy logic output

For a single case this section will now analyse the computed results and compare them with the error metrics and the goodness output computed by the fuzzy logic system. Figure 10 illustrates the validation plots produced for exemplary case L11A of Liu [59], and associated values of error metrics and the G output metric.

The predicted gas void fraction profiles show a generally good shape, 463 both the baseline and the computed profile. This generally good agreement 464 with the experiment is well represented by high values of the PCC. The 465 result with the Hessenkemper lift appears slightly deteriorated due to a shift 466 of the wall peak towards the wall, which is well captured by a drop of the 467 respective PCC. There are no significant changes in MRE. The drop in 468 overall goodness and a negative ΔG reflect the subjective evaluation of the 469 gas void fraction profiles. 470

The profiles for the turbulent kinetic energy are examples of curves with distinctively different shapes compared to the experimental data (wall-peak vs. core-peak). This judgement is well captured by very low values for the PCC, as well as very high values for the MRE. Comparing the baseline result to the new model no significant changes are observed. Consequently, the ΔG computed by the fuzzy logic system is relatively small.

The profiles for the liquid velocity show a good agreement with the experiment in terms of the shape. The difference to the experimental data slightly increases with the new model, as correctly captured by the *MRE* metric.

All the resulting G values of the validation fields are averaged to produce one value for the overall goodness of the CFD predictions for the case. The difference in results between the two lift force models is expressed by the difference ΔG . For the L11A case the new lift model slightly decreases the overall G and deteriorates results, which corresponds to our judgement for the plots in Figure 10.



Figure 10: Goodness evaluation for the validation fields of case L11A.

486 5.3. Overview of all case evaluations

The above evaluation of results expressed via the G metric is performed for each of the cases under investigation. Figure 11 illustrates the overall goodness values of all cases, represented as bars ranging from zero to one. Numbers next to each case indicate in green the cases which have improved, ⁴⁹¹ and in red the deteriorated ones, such as L11A on the top. A ΔG value ⁴⁹² averaged over all cases aims to quantify the general trend in results. Thus, ⁴⁹³ the plot allows to obtain a first overview of the general performance of a new ⁴⁹⁴ model.



Figure 11: Plots for the overall goodness of all 36 demonstration cases. Light blue bars represent the reference solution obtained with the baseline lift model, deep blue bars the solution obtained with the new lift model. Numbers next to each case indicate the difference in overall goodness, with red indicating a deterioration and green an improvement of results.

Similar plots are produced for the individual validation fields, such as the gas void fraction plot presented in Figure 12. The goodness values are based on the computed mean relative errors and Pearson correlation coefficients illustrated in Figure 13.



Figure 12: Goodness output for the gas void fraction prediction of all 36 demonstration cases.

Plots visualizing the change in goodness for each case, such as the ones 499 above, have proven to be a useful tool for analysing the performance of a new 500 model. Not only do they provide a neat case-by-case overview of results, 501 but also help pointing the researcher to the cases most affected by a new 502 model. Figure 12 indicates a slight change of gas void fraction results for 503 case L11A, but a more substantial change for case fullyDeveloped_39. This 504 is confirmed by the corresponding plots in Figure 2. Table 5 illustrates the 505 detailed input and output metrics for both cases, with the quality of CFD 506 predictions adequately quantified by the fuzzy logic system. 507



Figure 13: Computed error metrics for the gas void fraction prediction of all 36 demonstration cases. Top: Mean relative error. Bottom: Pearson correlation coefficient.

	fd_39	L11A					
	0.025 0.02 0.015 0.015 0.015 0.005 0.005 0.005 0.005 0.005 0.005 0.005 0.005 0.005 0.015 0.015 0.02 0.025 0.02 0.02 0.02 0.02 0.02 0.	0.4 0.3 0.3 0.25 0.2 0.25 0.1 0.05 0.0 0.2 0.4 0.6 0.8 1					
Baseline							
MRE	0.188	0.089					
PCC	0.287	0.701					
G	0.546	0.713					
New model							
MRE	0.585	0.091					
PCC	-0.822	0.349					
G	0.273	0.651					
$\Delta \mathbf{G}$	-0.273	-0.062					

Table 5: Comparison of the computed fuzzy logic metrics for the gas void fraction profiles in Figure 2.

The presented fuzzy logic plots above are a powerful tool assisting in 508 the model evaluation and comparison for the baseline model development 509 using a large number of cases. Note, however, that results will not cease 510 to require the careful interpretation by the experienced researcher taking 511 into account the underlying physical phenomena. An obvious limitation of 512 the current validation strategy is that bubbly flow cases typically require a 513 set of interdependent closures rather than isolated, individual models. This 514 means the computed error metrics and corresponding goodness evaluation 515 is only able to demonstrate the accuracy of all closure models combined. 516 How well each individual closure model performs remains a task of careful 517 interpretation by the investigator. 518

For a more detailed analysis of a new closure model the researcher can facilitate the keywords presented in Table 2, which are assigned to each subcase. Via keyword selection during the configuration step of the workflow
the model analysis can be tailored to specific cases of interest with certain
features.

The fuzzy logic analysis demonstrated here constitutes a first step towards 524 a more automated model evaluation. In the future a more refined control of 525 the results is possible by introducing alternative and/or additional metrics. 526 Furthermore, core and near-wall regions could be analysed separately adopt-527 ing different error metrics and fuzzy sets for these individual flow regions 528 if needed. The optimal use of fuzzy sets and metric combinations will be 529 determined by the expert community and will evolve by gaining experience 530 over time. 531

532 6. Conclusions

The development of closure models that can predict the behaviour of 533 multiphase flows continues to be a challenge due to the increasing number of 534 available model options, and their intricately-linked interactions. The base-535 line strategy offers a way towards a more sustainable model development. By 536 setting the goal of establishing a fixed set of models and related model con-537 stants it is turning away from case-specific tuning, and instead gives priority 538 to the generality and predictive capabilities of models. The practical imple-539 mentation of such a strategy involves the continuous validation of a large 540 number of cases available in the literature, which continues to grow. Within 541 the last few years of baseline research the HZDR team has accumulated a 542 diverse set of such validation cases and built an extensive case collection. 543

We have presented here a Snakemake workflow that now allows the flexible and fully-automated pre-processing, simulation and post-processing of all these OpenFOAM cases at scale. The automated production of hundreds of validation plots and their representation in a single, easily accessible webreport allow an efficient analysis of our CFD results and their comparison to the experimental validation data.

Such advanced case management enables us to integrate artificial intelli-550 gence tools that assist in the analysis and evaluation of the extensive amount 551 of results. The work presented here introduces a fuzzy logic controller quan-552 tifying the agreement of computed CFD results with the validation data. 553 By comparing new results with a reference solution obtained with the base-554 line model set this fuzzy logic tool allows the systematic evaluation of new 555 Euler-Euler models. The testing of a new lift force correlation demonstrates 556 the potential of such an approach with comprehensive plots illustrating neat 557 case-by-case comparisons of the accuracy of the CFD predictions. 558

The further development of the fuzzy logic evaluation and its extension by 559 more input metrics is ongoing. A particular focus will be on metrics describ-560 ing the convergence behaviour and runtime performance of cases to obtain 561 an alternative criteria by which to compare various Euler-Euler models. Fur-562 thermore, the uncertainty of the validation data should be included into the 563 evaluation. The application of fuzzy logic is just one of many potential ways 564 of including data science tools into the baseline model development. Another 565 valuable area of further work is the integration of case-specific keywords into 566 the model evaluation for further categorisation, which suits various machine 567 learning algorithms. 568

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