SYNTHESIS OF THE OECD/NEA-PSI CFD BENCHMARK EXERCISE

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ABSTRACT

The third International Benchmark Exercise (IBE-3) conducted under the auspices of OECD/NEA is based on the comparison of blind CFD simulations with experimental data addressing the erosion of a stratified gas layer by a buoyant jet in a large vessel. The main objective of the activity was to evaluate the use of CFD for simulating flow mixing in a model containment volume for conditions of practical interest to nuclear reactor safety. This numerical benchmark exercise is based on a dedicated experiment carried out in the PANDA facility at the Paul Scherrer Institut (PSI) in Switzerland. The use of non-prototypical fluids (i.e. helium as simulant for hydrogen, and air as simulant for steam), and the consequent absence of the complex physical effects associated with steam condensation enhanced the suitability of the data for CFD validation purposes. Blind calculation results were submitted by nineteen (19) participants, and the results have been analysed and compared with the experimental data by the PSI team to prepare a synthesis, the main results from which are summarized in the present paper.

KEYWORDS
Containment, stratification erosion, buoyant jet, benchmark, OECD/NEA

1. INTRODUCTION

As part of an ongoing commitment to extend the assessment database for the application of CFD to nuclear reactor safety issues, a *Special CFD Group* has been formed within the scope of activities of the OECD/NEA[‡] Working Group on the Analysis and Management of Accidents (WGAMA). The organization of *blind* international numerical benchmarking exercises is one of the most important tasks of this group [1]. The first such exercise was launched in 2009, and aimed at testing the ability of state-of-the-art CFD codes to predict the important flow parameters affecting high-cycle thermal fatigue induced by turbulent mixing in a T-junction [2]. The second in the series aimed at testing the ability of the codes to predict the degree of mixing downstream of a spacer grid in a fuel bundle geometry [3]. For the third exercise, reported in this article, the topic of gas mixing in containment in the presence of hydrogen under initially stratified conditions has been selected. This choice derives from the need to quantitatively assess the potential of the hydrogen, generated during a severe accident following core degradation, to form an explosive mixture in the upper part of the containment, and the subsequent penetration and erosion of this hydrogen-rich layer induced by buoyant jets rising from beneath. The 3-D nature of the flow generated invites the use of CFD (or CFD-type) approaches, but such applications are often restricted by the lack of adequate validation data of the basic physical phenomena at an appropriate scale. The benchmark aimed

[‡]*Organisation for Economic Cooperation and Development, Nuclear Energy Agency*

to provide invaluable data in the quest to improve the reliability of numerical simulation approaches in such situations. The recent accident at the Fukushima Daiichi complex in Japan in March 2011 has refocused attention on this issue globally.

This third International Benchmark Exercise (IBE-3), again conducted under the auspices of OECD/NEA, is based on the comparison of blind CFD simulations with experimental data addressing the scenario described above. The numerical benchmark exercise is based on a dedicated experiment performed in the PANDA facility at the Paul Scherrer Institut (PSI) in Switzerland [4], and is designed to investigate the gradual erosion of a helium-air layer at the top of a free volume caused by a low-momentum air/helium jet emerging at a lower elevation.

The use of non-prototypical fluids (i.e. helium as simulant for hydrogen, and air as simulant for steam), and the consequent absence of complex physical effects produced by steam condensation, enhanced the suitability of the data for CFD validation purposes. In consideration of the scope of the synthesis, and the availability of a detailed description of the experiment used for IBE-3 [4], this paper includes only a brief description of the experiment and the few data that were used for the comparison with the submissions. For a complete presentation of the experimental results, the reader is referred to [4]. The complete synthesis [5] was presented at the CFD4NRS-5 workshop, and will be included in a draft report currently in preparation [1], to be submitted during 2015 to the CSNI[#] for review and approval.

Adopting the format of the reports for the two previous benchmark exercises in this series, this full report also includes a ranking of the contributions, where the largest weight is given to the time progression of the erosion of the helium-rich layer. Due to space limitations, the present paper does not include any details of the ranking process, but instead is restricted to the essential outcomes of the synthesis.

2. ORGANISATIONAL ASPECTS

The organising committee was formed from the current members of the *CFD Bureau* at the time, together with the member of the PSI team who would perform the synthesis of results (M. Andreani). Table I lists the members of the committee, their affiliations, and their principal functions within the scope of this benchmark exercise.

Table I: Members of the OECD/NEA–PSI containment CFD benchmark organising committee.

Brian L. Smith	PSI, Switzerland	Chairman
Michele Andreani	PSI, Switzerland	To perform synthesis of results
Dominique Bestion	CEA, France	Expert, and special advisor on workshop organisation
Ghani Zigh	US NRC, USA	Expert on modelling containment fires
Martin Kissane	OECD/NEA, France	Secretariat

The kick-off meeting of the benchmark exercise (25 April, 2013) took place at the NEA Headquarters in Paris. In total, 49 registrations were made from organisations from 17 countries. Table II lists the countries specifically, and the number of registrations per country. All registered participants subsequently received the official benchmark specifications. The kick-off meeting was attended by 26 delegates, from 11 countries, plus 8 observers. The final timetable for the activity is given in Table III. The Final Benchmark Specifications document was distributed on August 28, 2013. This gave

[#] Committee for the Safety of Nuclear Installations participants around nine months to complete their calculations, and to submit their numerical results by the deadline date of May 30, 2014.

Table II: Registrations to the OECD/NEA–PSI containment CFD benchmark.

China†	1	Italy	6	Spain	3
Finland	1	Japan	3	Sweden	1
France	10	S. Korea	1	Switzerland	4
Germany	3	Romania	1	UK	2
Greece	1	Russia	7	USA	3
Hungary	1	Slovenia	1		

† By special permission, China not yet having the status of being an official member of the OECD.

Table III: Timetable for the OECD/NEA–PSI CFD containment benchmark.

April 25, 2013	Kick-Off Meeting
May 31, 2013	Distribution of a provisional version of the Benchmark Specifications (geometry plus range of flow parameters)
July 31, 2013	Distribution of draft version of the Benchmark Specifications (geometry plus precise flow parameters)
August 15, 2013	Deadline for comment/queries from participants concerning the Benchmark Specifications to be returned to the organisers
August 28, 2013	Distribution of the final version of the Benchmark Specifications
May 30, 2014	Deadline (NOT EXTENDED) for receipt of simulation results
June 4, 2014	Open Benchmark Meeting (first opening of the test data)
Sept. 10, 2014	Presentation of results, and synthesis, at the CFD4NRS-5 Workshop (ETHZ, Zurich, Switzerland)

Participants were encouraged to upload their data files (as well as essential information on the mesh and physical models they had employed) to a dedicated PSI ftp site. In return for their participation, they would receive the test data from the benchmark experiment in full. Apart from a number of users with observer status on the site, of the 49 who originally registered interest in participating in the benchmark activity, 29 officially requested a username and password on the ftp site.

Also, it was made clear from the outset (i.e. at the *Kick-Off Meeting*) that only one set of blind numerical predictions would be accepted by the organisers from each participant. The organisers wanted each participant to submit what he/she considered to be their “best” numerical predictions. In total (after removing one or two incomplete data sets), 19 submissions were received by the deadline, and these formed the basis of the synthesis procedure subsequently carried out by PSI, and reported at the CFD4NRS-5 Workshop [5].

3. THE EXPERIMENT

3.1 Geometrical Configuration

The PANDA facility is a multi-compartment, large-scale thermal-hydraulics test rig located at the Paul Scherrer Institut (PSI), Switzerland [4]. Specifically for this CFD benchmark experiment, one test vessel had been isolated from the others, and this constituted the test section (Fig. 1). The test vessel, 8 m in height, is composed of four sections, each of 4 m outer diameter but with varying inner diameters, depending on the local wall thickness. At the top of the test vessel, there is a 980 mm diameter manhole; its presence adds an extra 464 mm to the vessel internal height. All the sections are made from stainless steel. The total enclosed volume within the vessel is 90.24 m^3, and the total internal surface area is 108.49 m^2. For this test, a vertical injection line, with internal diameter 75.3 mm and wall thickness 3.6 mm, was placed off-center, at a horizontal distance of 647.5 mm (nominally 650 mm) from the axis of the test vessel. The outlet from this injection line is located 2995 mm (nominally 3000 mm) above the lowest point on the axis of the vessel, and is positioned vertically, to produce a jet directed upwards. The straight section of the inlet pipe upstream from the outlet orifice is more than 30 diameters in length.

In order to keep the pressure constant, the air/helium mixture in the vessel is vented to atmosphere via a funnel, oriented downwards (red component in Fig. 1) located just above (maximum gap ~160 mm) the base of the vessel. For convenience, the venting is made via the large interconnecting pipe (IP in Fig. 1), which had been blocked off especially for this test. Details of the geometry (including technical drawings and CAD files) were included in the technical documentation distributed to the benchmark participants.

3.2 Initial and Boundary Conditions

The experiment addressed the mixing produced by a vertical jet in a vessel where stratified conditions existed before the start of the gas injection. A helium-lean mixture of air and helium was thus injected into the vessel, where initially a helium-rich layer occupied the upper region, and pure air filled the volume below (Fig. 1). The experiment was conducted under ambient conditions: i.e. at nominal atmospheric pressure. The gases in the vessel were nominally at room temperature, and the temperature of the injected air/helium mixture was slightly elevated. The test was carried out at ambient temperature (nominally 20^{o}C), except for the slightly elevated temperature of the incoming air/helium mixture at the injection pipe outlet. Consequently, the heat losses from the external surfaces of the test vessel in this test are considered to be small over the duration of the transient (2 hrs.).

Prior to the test, stratified air/helium conditions had been created in the test vessel. A helium-rich layer occupied the region h > 6000 mm, air filled the region below 5000 mm, with a transition layer existing between these levels. The measured helium and air molar fractions at time t = 0 as a function of elevation are also displayed in Fig. 1. All concentration measurements are subject to total combined uncertainties of < 1%. The initial gas temperatures were between 20.5 and 22.5^{o}C, with the helium-rich layer being generally cooler than the region below. The wall temperatures were also measured, in the range between 21.6 and 23.2^{o}C, all temperature measurements being subject to an uncertainty of ± 0.7 ^{o}C.

The total volumetric flow rates of helium and air through the injection line were monitored continuously during the test, and remained constant for the test duration. The mass flow rates of air and helium were 21.52 g/s and 0.42 g/s, respectively. Injection molar fractions and temperature were measured 36 mm above the injection line exit. The molar fractions of helium, air and water vapour were constant, at 0.134, 0.862 and 0.004, respectively. The temperature increased with time, being initially 20^{o}C, and rising to 29.3^{o}C at the end of the transient.

The velocity conditions at the outlet of the injection line were determined by PIV measurements in a separate, ex-vessel test; details of the profiles were given in the technical specifications. From the measured instantaneous velocity components, mean and root-mean-square (RMS) values of the pipe exit velocity data were calculated. Details are given in [4]. All data were provided in graphical and tabular form to the benchmark participants.

3.3 Measurements

In this benchmark, selected time-dependent measurements for mass concentration and temperature were made available for comparison [4]. Additionally, the vertical component of the velocities, as well as the corresponding RMS values of this component, were also used in the comparison between measurement and calculation, at specific times, and along specified horizontal and vertical lines. The sampling period for the helium, air and water vapour mass concentrations at the inlet to the PANDA vessel (pipe exit) and at the outlet (exit of the vent line) was 30 s. These same quantities were also recorded at 19 other locations in the vessel. The sampling period for these lines was 226 s.

The K-type thermocouples (TCs), each of 1.0 mm diameter (frequency response 0.5 Hz), had been placed at strategic locations in the PANDA vessel relevant to this test, many in the line of the jet issuing from the injection pipe. Temperature measurements were taken at 218 locations, though only selected temperature data had been requested by the benchmark organizers. Mean velocities and velocity fluctuations were measured using PIV in three regions of the flow (see below), all above and around the axis of the injection pipe. These measurements were subsequently processed to produce averaged values over a time period of 204.6 s.

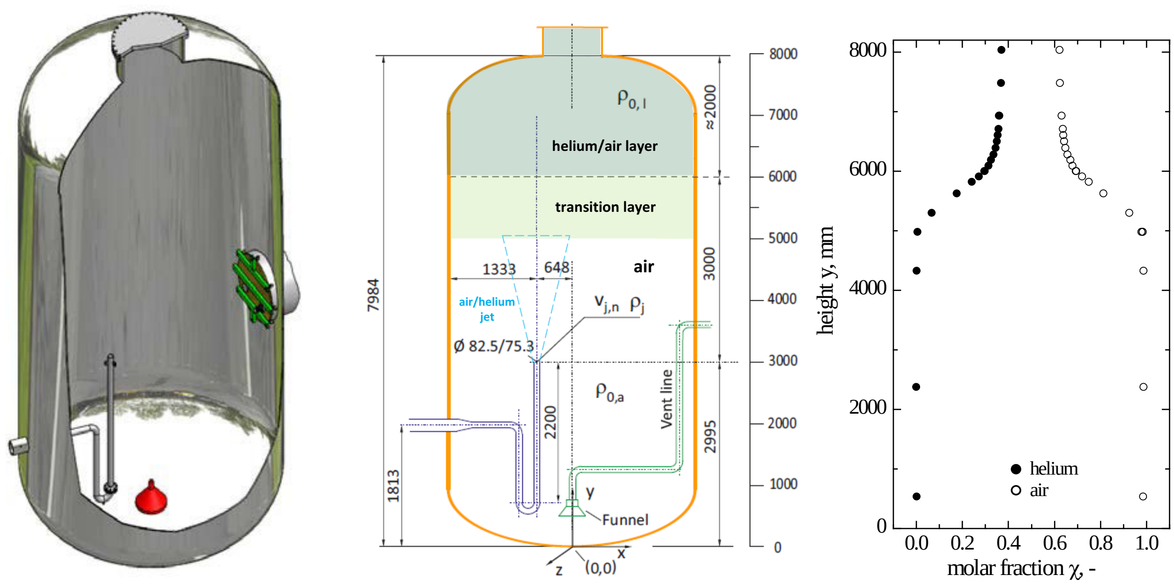


Figure 1. Geometrical Configuration for the Experiment and Initial Gas Distribution.

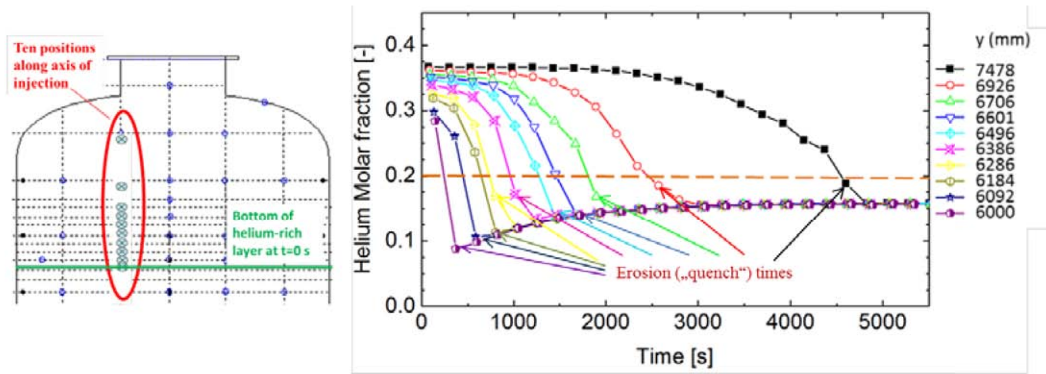
3.4 Calculated variables to compare with experimental data

The main interest of the exercise is to evaluate the capability of the codes to simulate:

a) the erosion rate of the helium-rich layer;
b) the global mixing in the vessel.

The erosion process is described by the sequential drop of helium concentration (below a specified value) at increasing elevations along the injection line: this value was chosen to be 0.2. Ten sampling lines locations were chosen to characterise the history of the mixing above the injection pipe. These positions are shown in Fig. 2a. The time histories of the measured helium concentrations at these locations are shown in Fig. 2b, where the "quench" times are also indicated. As the scanning time was 226 s, the uncertainty of the "quench" times is negative (-226 s), as the reduction below 0.2 can only occur earlier.

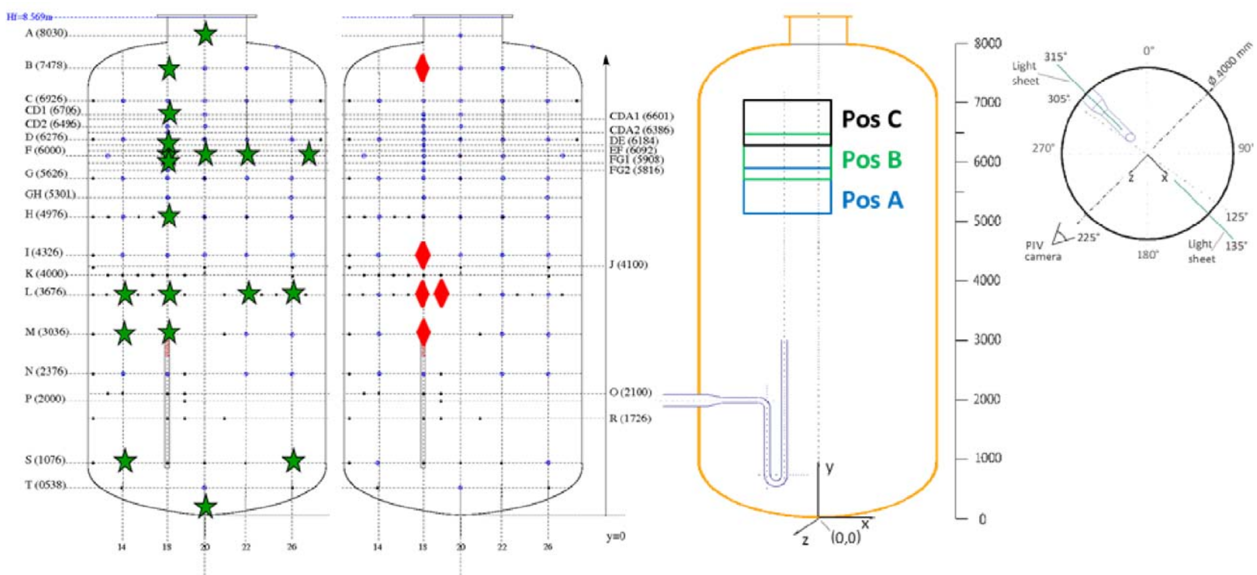
The global mixing can be evaluated considering the time history of the helium concentrations at measurement positions distributed over the entire vessel, including some along the injection line. Figure 3a shows the positions of the measurements used in the present benchmark test. Among the many temperature measurements available, only five were selected for the benchmark (Fig. 3b). Due to space limitations, the results of the temperature predictions will not be presented in this paper. The full discussion of these variables is included in [5].



a) b)

Figure 2. Positions of Concentration Measurements used for Evaluating the Stratification Erosion (a); and Time Histories of Helium Concentration at those Positions (b).

Additionally, seven vertical and horizontal profiles of the mean vertical velocity distribution, and the RMS values of the vertical velocity fluctuations, were requested at three times; these to be compared with the values measured using PIV in windows (Fields-of-view, FOVs) at three positions (A, B, and C in Fig. 3c). The vertical distributions of turbulent kinetic energy (TKE) along the injection axis at three specified times were also requested.



a) **b)** **c)**

Figure 3. Positions of: Concentration Measurements used for Evaluating the Global Mixing (a); Temperature Measurements Used for the Benchmark (b); PIV Fields-Of-View (FOVs) (c).

4. SUMMARY OF THE SUBMISSIONS AND MAIN RESULTS

4.1 Summary of the Submissions

Nineteen submissions have been received. They are summarised in Table IV. The entries only address the main features of the physical models, mesh and simulation times. The few details on the numerical methods used that were asked for are not included here. It is noted that:

- Mostly commercial codes (CFX, FLUENT, STAR-CD) were used. A few submissions used "in-house" CFD codes, and two used a containment code with CFD capabilities (GOTHIC). Finally, one participant used an open source CFD code (OpenFOAM).
- None of the meshes used are impressively fine. The number of cells ranges between 4000 and 4.3 million. It is left to the individual participants to further clarify these important choices. Especially for simulations using LES for representing turbulence, the use of large cells should be critically evaluated.
- Approximately half the participants used standard URANS turbulence modelling approaches, i.e. variants of the well-established k-ε model, in connection with a mesh that was aimed to resolve the prevailing flow structures (between 400 000 and 2.2 million cells). The other half used refined turbulence models (LES, SAS, RSM), or standard modelling on a coarse mesh. For clarity of presentation, the contributions in these two classes of submissions (standard turbulence models and "others") are distinguished in the discussion of the main results.
- Nearly all participants were able complete the simulation (7200 s), although at the cost of very large "equivalent" CPU time (referred to a single processor), which for LES simulations would amount to several years on a single processor, in spite of all the simplifications adopted for this particular benchmark exercise. These times, together with the fact that some users could not complete the simulation, shows how demanding a simulation of a typical flow of interest for containment applications still represents. The prevailing exorbitant costs of CFD with a large number of meshes over long simulation times maintain the interest in evaluating the continued use of approaches involving much coarser meshes.
- The modelling of the injection pipe, and of the flow outlet conditions, is quite different for the various simulations. As regards the average turbulence intensity at the pipe outlet, this varies over a surprisingly broad range, given the supplied information: between 0 and 20%. Considering the spread of the results for some variables portraying the spatial evolution of the flow above the injection, it is suggested here that the representation of the pipe, and the flow exit conditions, should be carefully considered in any further studies.
- The values of the turbulent Schmidt number ranged between 0.7 and 1. Nearly all participants used values for the molecular diffusivity close to 7×10^{-5} m^2/s^2, which is frequently quoted in the technical literature. Four users, however, used smaller values, or zero. Thus, it is suggested here that future sensitivity studies should include investigations on the importance of these two parameters.
- Many users did not consider heat transfer between the gases in the vessel and the vessel walls. Since the temperature differences within the fluid domain are very small (less than 10 K), it is reasonable to assume that specific modelling of heat transfer would not affect the evolution of the helium concentrations and velocities. Nevertheless, the results submitted for the temperatures would then be invalid, as a result of the gradual warming of the gases in the vessel.

4.2 Main results from all submissions

In this paragraph, the main results from all submissions are compared with the experimental data up to 4000 s (the time at which the helium concentration at the uppermost elevation along the injection line dropped below the chosen threshold value of 0.2). The results, for clarity of presentation, are subdivided

Table IV: Summary of the submissions (grey shaded: Group 1 submissions, using variants of the k-ε model and a sufficiently detailed mesh; not shaded: Groups 2 submissions, using other turbulence models or a very coarse mesh).

User	Code	Turbulence model	Nr. Cells $\times 10^3$	Gas to wall heat transfer	Sc_t	D_{AB} (m^2/s) $\times 10^{-5}$	Inlet pipe		Simulation time (s)	Equi-valent CPU time (hours)
							Mo-delled (Wall/ Fluid)	Tu Outlet (%)		
1	Trio_U 1.6.8	k-ε	2900	NO	0.7	7	NO	7	2100	105800
6	P^2REMICS	k-ε	1383	NO	1	7	NO	10	7535	3024
8	CFX 14.5	SST	717		1	N/A			6981	13444
11	CFX 15	k-ω SST	2200	YES	0.9	7.2	YES	8	5272	4960
12	FLUENT 14	RSM	2077	NO	0.7	7.13	NO	5	7200	1800
17	FLUENT 14.5	k-ω SST	2200	YES	0.7	7	N/Y	5	7200	576
19	STAR-CD 4.20	Low-Reynolds k-ε	2064	NO	0.9	6.7	YES	8	7200	68608
20	CFX-14.5.7	k-ω SST	1612	YES	0.9	Corre-lation	YES	5^+	4437	20164
32	FLUENT 12.1.2	k-ε (realizable)	474	YES	0.7	8	N/Y	13	7200	6960
33	CFX 14.5	SAS-SST	1263	YES	1	=bulk viscosity		7.3	8000	11680
34	CABARET 2.5	ILES	4331	NO	N/A	1.83/ 1.86	NO		7200	49152
37	OpenFOAM 2.1.1	Modified k-ε	2035	NO	1	Corre-lation	NO	1.56	10500	258048
38	Logos 4.0.7	Laminar	300		N/A	N/A		N/A	~ 3000	N/A
39	CFX 14.5	SAS-SST	1203	NO	0.9	7.2	Y/N	5	7200	7392
41	FLUENT 15	k-ε	448	NO	0.7	2.88	Y/N	11.8	7200	6600
42	FLUENT 15	LES (dyn. Smagorinsky)	790		0.7	Kin. theory	YES	N/A	7200	118440
43	FLUENT 14	ZLES/ WALE	1626	YES	0.7	Kin. theory	YES	20	2000	145152
45	GOTHIC 8.0(QA)	k-ε	4	NO	0.7	2.88		0	7000	3
47	GOTHIC 8.0(QA)	k-ε in jet region, Mixing length elsewhere	8	NO	(1)	0	NO	0	7200	48

in two groups, namely the results of simulations using variants of the k-ε turbulence model and "typical CFD meshes", and the "others". The simulations are labelled according to User number, turbulence model employed, and the number of cells adopted (in millions). Submission U38 included only a few results, and therefore this contribution will not appear in the comparison plots. Figure 4 shows the times at which the helium concentration drops below the 0.2 level at the ten selected elevations along the injection pipe axis. For both groups of calculations, the spread of the results is disturbingly large. It is worth noting that:

- One simulation (U33) predicts the erosion times nearly perfectly. Three simulations (U6, U37, U12) do not predict the drop to 0.2 at the highest elevation within the simulation time, and two (U8, U34) strongly overpredict the time of this occurrence (which the two participants extrapolated from the previous time history of the concentration, so the errors could thus be even larger than those shown in the Figure). For these cases, the upwards penetration of the jet was too slow. All others overpredict the mixing, to various extents.
- The spread of results obtained with variants of the k-ε model (Fig. 4, left) is also quite large. It is especially interesting to note that one of the simulations (U17) using the SST turbulence model

produces results notably different from other two simulations, U11 and U20, for which the same turbulence model had been employed, and similar mesh concentrations (from 1.6 to 2.2 million cells).

- It should be noted that the two best submissions (U33 and U11) based on all results [5] were obtained using the CFX code. It would be interesting if a user could run the simulation with the same model choices and mesh, but with the two codes (e.g. CFX and FLUENT), to check whether certain results depended on the solver used (and the way "control volumes" are defined in the two codes) and/or on the numerical parameters selected.
- Although the most accurate simulations employed the SST and the SAS turbulence models, it is not obvious that they should be considered superior to the standard k-ε model, because this latter model was either used in association with a coarser mesh or in the framework of in-house codes, for which the validation is certainly not as extensive as for the commercial codes. Moreover, the participants who submitted the successful results using the SST model were all familiar with previous tests in PANDA.
- All LES simulations produced from poor to very poor results. The use of LES with coarse meshes is anyway rather questionable. These results suggest that accurate simulations for the long transients of interest for containment analysis using this advanced turbulence modelling approach are not yet affordable. The best predictions seem to be obtained by the two simulations using the SAS-SST model. It will be shown below, however, that this holds true for U33, but the outwardly impressive results of U39 in Fig. 4 (right) could be misleading.
- Surprisingly enough, very good results (U47) were also obtained using the GOTHIC code with a very coarse mesh (8000 cells). The much worse results obtained by the second GOTHIC user (U45) show the strong dependence of success of such coarse-mesh approaches on the user.

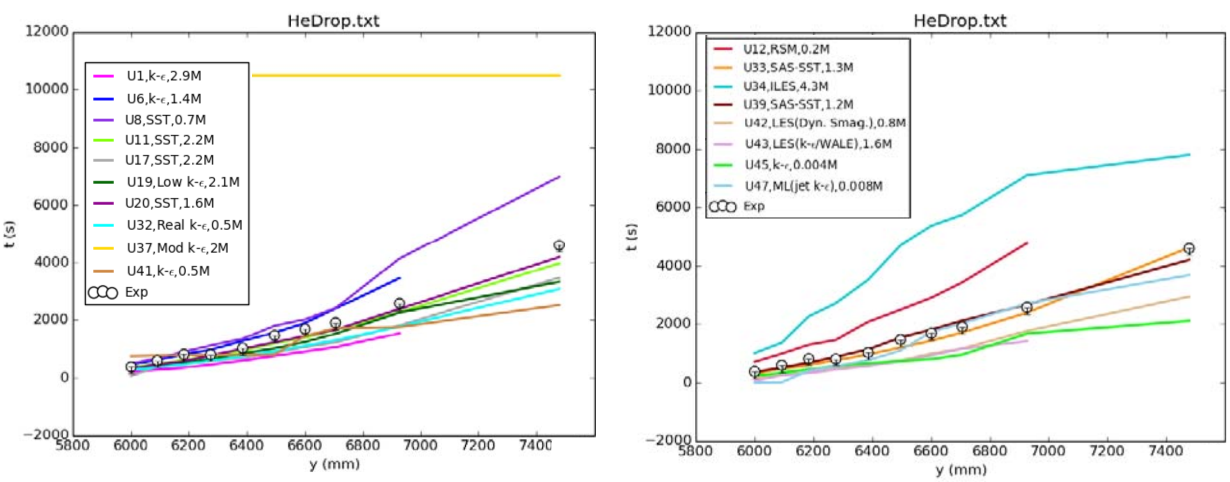


Figure 4. Times of Helium Concentration drop below 0.2 at various Elevations along Injection Line. Left: Group 1; Right: Group 2 (see Table IV) .

With regard to the global mixing, the time histories at one position outside the jet axis in the upper part of the vessel and close to the bottom of the vessel, are considered for illustrating qualitatively the performance of the various codes/models. Figure 5 shows the calculated and experimental results for the two groups of simulations. Most simulations using variants of the k-ε model predict reasonably well the mixing outside the jet, and the time of propagation of helium down to the vent. Only one submission (U37) displays completely wrong results, and one user (U41) obtained good agreement at some positions, but large discrepancies at other locations. In particular, U41 predicted a premature propagation of helium into the lower head, indicating a too fast mixing process.

It is interesting to note that the nearly constant value (increasing very slowly) of the helium concentration at the bottom of the vessel (Fig. 5, MS_17.txt) in the last period (t > 4000 s) of the transient was captured only by two users (U6, U8), whereas all other simulations predict a maximum, followed by a slow decrease, a behaviour which is difficult to explain.

The simulations of the second group also display some interesting characteristics:

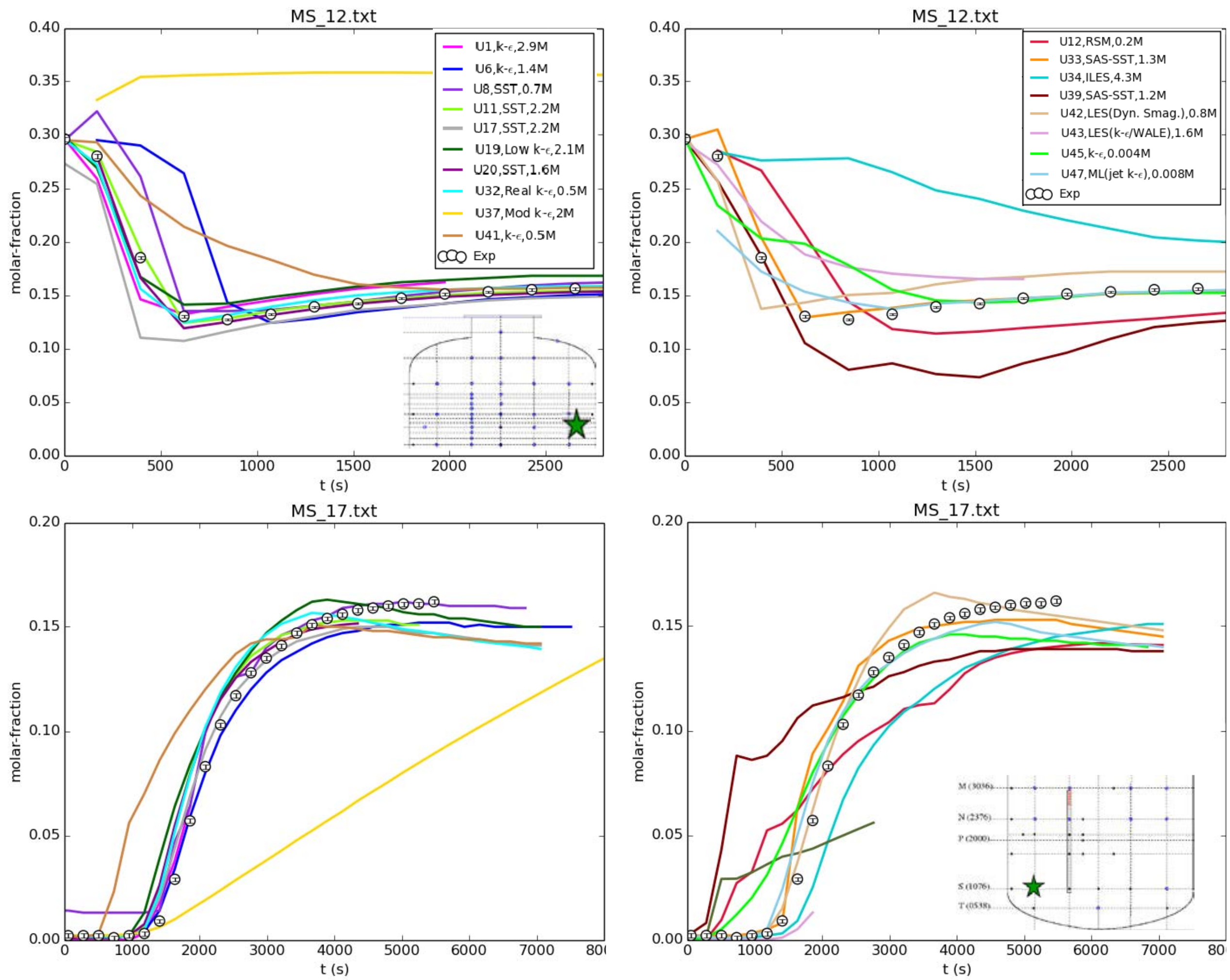


Figure 5. Helium Concentration Time Histories at one Position (z=6 m) outside the Jet (Top); and close to the Vent Inlet (Bottom).

- The LES simulations again give very different results, with reasonable agreement against experiment obtained only by one user (U42), although this submission overpredicts the equilibrium helium concentrations at all measured locations.
- One of the two simulations using the SAS model (U33) shows excellent agreement with the test data, although the trend at the lowest elevation is less monotonic than seen in the experiment. In particular, a sudden delayed increase is observed at the time when helium arrives into the lower head. U33 is also the only submission, among those correctly reproducing the general trend, which captures also the nearly constant value of the helium concentration at the end of the transient at this location.

- The other simulation using SAS (U39), which seemingly predicted the upper layer erosion process quite well, displays a completely unphysical helium concentration evolution at all three positions. Considering the small differences between the mesh and physical parameters adopted by User U39 to those of U33, it is difficult to identify which are the differences in the simulation set-up that would result in such different predictions. From the information provided, it appears that both participants used second-order methods, but User U33 adopted stricter convergence criteria than User U39, and ran the simulation on a 64-bit machine rather than on one with 32-bit precision. The investigation of whether convergence criteria and arithmetic precision can be responsible for the dramatically different results will be an interesting aspect of any future analyses, an exercise which is left to the individual participants.
- Coarse-mesh simulations seem to be capable of capturing the global mixing, with results comparable to those obtained with meshes composed of a number of cells between two and three orders of magnitude higher.

The differences in the calculated erosion rates can partly be explained by the different space evolution of the vertical velocity at the requested times.

Figure 6 shows the vertical distribution of the y-component of the velocity along the injection axis at time t = 111 s in the region of the PIV window (Pos.A, between 5000 and 5600 mm). At this time, considering that the helium concentration distribution had not yet had time to change appreciably, the PIV window can be assumed to be fully lined up with the transition region, where the helium concentration increases from values close to zero to about 20%. It is thus reasonable to assume that, at this early stage in the transient, the velocity at the bottom of the PIV region should be close to that for a free, round jet (range of expected values in Fig. 6), as calculated by means of standard correlations [6]. Therefore, it is quite surprising that only one submission of the first group (U19) accurately predicts the vertical velocity at this location, whereas most of the others, which were successful in predicting the erosion rate (Fig. 4), underpredict the velocity. It is also noted that the largest discrepancy (between calculation and experiment) amounts to around 40%, which for CFD simulations of a free jet is an unacceptable result. For this group (with the exception of U11, for which the discrepancy in the velocity is quite large), a correlation exists between the fidelity in predicting the velocity decay and the success in predicting the erosion rate.

The simulations of the second group show a similar dispersion of results, with the two submissions using the SAS model, and the two using LES with a subgrid model, reproducing the correct trend, and predicting the velocity at the top of the PIV window fairly well. One of the coarse-mesh simulations (U47) also produces comparably good results, whereas the simulations incorporating the ILES and RSM turbulence models, together with the other coarse-mesh simulation, badly fail to predict the correct velocities. Also in this case, a correlation exists between the success in the prediction of the erosion rate and the prediction of the central jet velocity for all calculations, except the two using LES, which underpredict the upward penetration of the jet into the helium-rich layer, but slightly overpredict the approach velocity.

Valuable insight into the unexpectedly large variation of results, and partly also as the cause of the contradicting results, is offered by the axial evolution of the turbulent kinetic energy (TKE), which is displayed in Fig. 6. With the exception of some submissions (for which the good prediction of the TKE did not result in a good simulation of the erosion process), generally the success of the predictions with regard to erosion times seems to be correlated to a good prediction of the TKE in the PIV region. The dispersion of the results, also for simulations using the same model and meshes of the same detail, is again quite disturbing, especially considering the near-field region, where, together with reasonable predictions of the evolutions, unphysical trends can be identified, with the position of the maximum outside the expected range (i.e. between 7.5 and 8.5 hydraulic diameters, according to [7]). The variation in results in the vicinity of the pipe exit strongly suggests that the modelling of the pipe, and strict implementation of the measured boundary conditions (profiles of velocity and turbulence intensity), may play an important role in determining the predicted capability of the jet to erode the upper layer; a fact that should be considered in any post-test analyses. Due to the similarity of the initial flow from the injection pipe to that of a free, round jet, it is suggested here that before any full simulation of the transient be attempted, the basic jet model, and all relevant parameters (including the numerical ones), should be verified by means of stand-alone simulations of the basic jet flow.

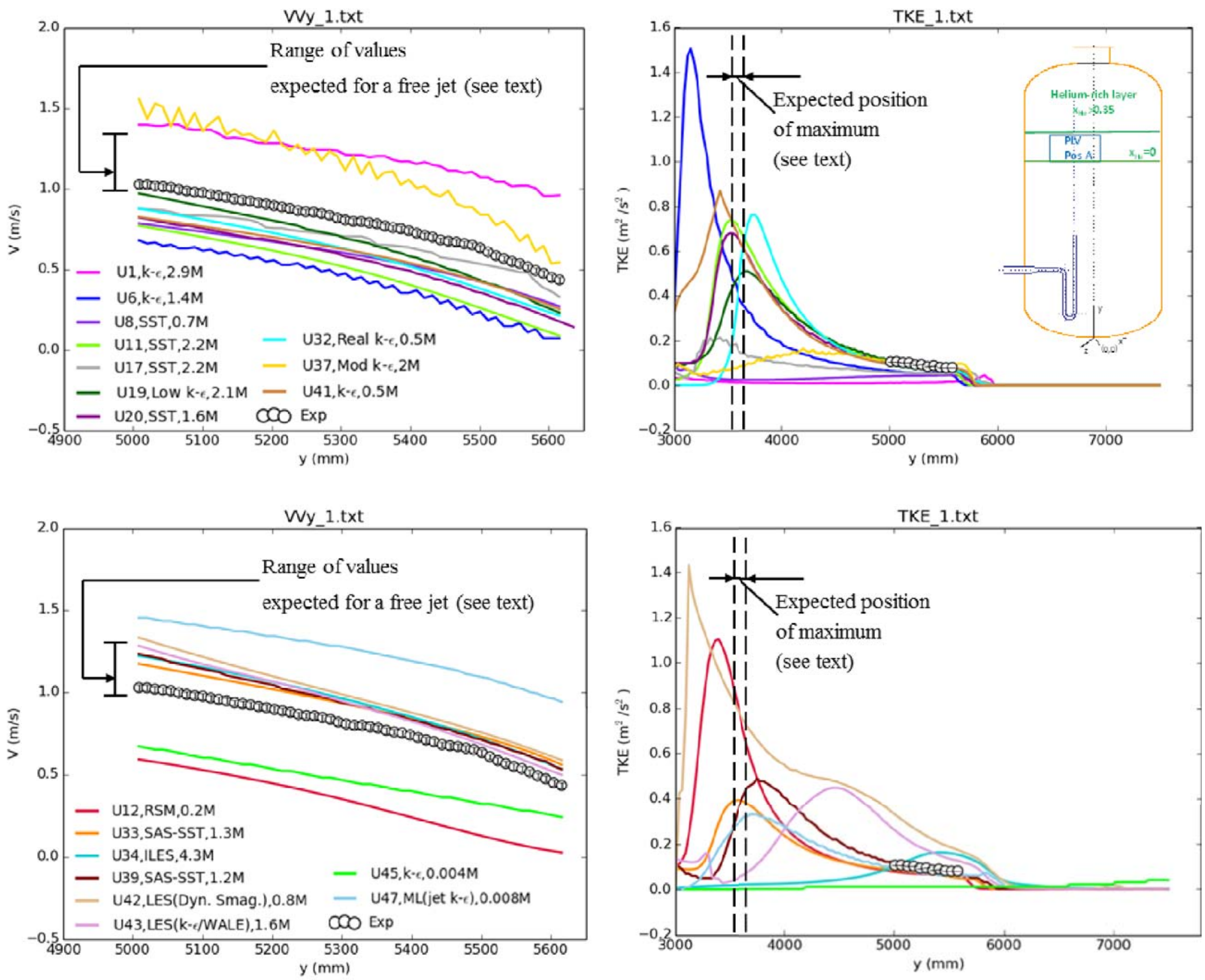


Figure 6. Vertical Distribution of the y-component of the Velocity along the Injection Axis at 111 s (left); Vertical Distribution of TKE along the same Vertical Line (right).

Some additional general considerations on the fidelity of the various simulations can be gained from a comparison of the calculated horizontal velocity profiles and gas temperatures [5]. Due to space limitations here, it is only noted here that a large spread of results exists in the calculated velocity profiles, with anomalous profiles of the RMS predicted by the most successful submission (U33, using SAS). Moreover, most of the simulations that correctly predicted the temperatures, and the temperature differences, were also among those that were successful in predicting the erosion rate (U11, U17, U20, U33, U47). In general, although it is unlikely that heat transfer played an important role in this test, it can be argued that the choice some users made not to model heat transfer to the walls is unwarranted, given the heat capacity of the wall material, and reflects the general issue that, for any modelling approach (including CFD), it is necessary to be able to identify all the processes of interest, and include them in the analysis.

5. CONCLUSIONS

The first general conclusion from this benchmark exercise, which is concerned with containment flows, and in particular the break-up of a stratified layer by jets issuing from beneath, is that, even for an over-simplified, basic flow configuration, a variety of results can be obtained from state-of-the-art numerical approaches, accompanied by an unexpectedly large spread in the principally predicted variables. In fact, the rate of the erosion of a helium-rich layer in this test was strongly over predicted in some simulations, and that a few simulations predicted the persistence of the stratification well beyond the time recorded for its break-up in the experiment, and in some cases exceeded the recommended simulation time (itself an over-estimate). This large spread in results, increasing with time into the transient, indicates that the set-up of a new problem (at least for those users who had never before simulated a similar experiment in the PANDA geometry) implies a certain risk in the choice of appropriate modelling approaches, which, perhaps, can only be avoided by commitment to some learning process in the simulation of such modelling situations.

Moreover, none of the submissions received was able to correctly predict all the variables requested. Hopefully, post-test analyses will identify the reasons for the failure of some simulations, the limited accuracy of most submissions, and some prevailing inconsistencies in those predictions judged to be the most successful. However, one important outcome of the exercise is that an established methodology for performing CFD simulations of a long transient, that is one of interest for containment safety analysis, does not yet exist. At the simulation level, the mesh resolution adopted by the various participants varied over a broad range, and, in the absence of any accompanying report to each submission, it is not clear how each participant arrived at the conclusion that their chosen mesh was adequate.

Obviously, in regard to turbulence modelling, a variety of choices had been expected, and the prevailing use of the most popular variants of the k-ε model had also been anticipated. However, other modelling choices and parameters were quite different between the various submissions, including how to model the injection, the most appropriate turbulent Schmidt number, and even the molecular diffusivity. The cumulative effect of all these choices is difficult to estimate without further calculation.

A few simulations predicted fairly well the overall transient behaviour, but the success of a particular calculation cannot be correlated with the choice of turbulence model as such. In fact, although the most accurate simulations had employed the SST and the SAS models, it is not obvious that they should be considered superior to the standard k-ε model in this context, because this latter model was either used in association with a coarser mesh, or in the framework of “in-house” or “open-source” codes, for which the validation database is certainly not as extensive as for the commercial codes.

The two predictions using the SAS model produced significantly different results, one of them totally missing the global mixing time, and predicting migration of helium to the bottom of the vessel after a very short time from the beginning of the transient, thousands of seconds before it was actually recorded in the test. Also, the fidelity of the predictions incorporating the SST model was different for the three submissions for which this model had been adopted although mesh, parameters, and other modelling choices, were apparently close to each other, and the participants using this model were all familiar with previous tests in PANDA.

It is also interesting to note that the accuracy of one coarse-mesh prediction (U47, which incorporated only 8000 cells) is comparable to that obtained by the best CFD predictions, at least with respect to the mixing of the initially stratified condition, at a fraction of the computational cost of the most accurate CFD simulations. Although this simulation used a combination of the k-ε model and the Mixing Length model for turbulence modelling, which could be considered unacceptable practice by the traditional CFD community, results from this benchmark do draw attention to the issue of a reasonable balance between accuracy and computational cost being maintained in studies of this type.

With regard to the performance of the LES simulations (three submissions), it can be definitely stated that it was far below expectations, the results being closer to the worst predictions using simpler turbulence models. Since the mesh used was definitely too coarse for this kind of modelling approach, and the CPU times an order of magnitude larger than for most RANS simulations, the only result from this exercise is that the use of LES in containment analysis is not yet affordable for the long transients of interest.

Another interesting result emerging from the inter-comparison of all the numerical simulations is the spread in the profiles of the vertical velocity and turbulent kinetic energy along the injection line, and the limited accuracy compared to measured values. This result suggests that, in simulations of this type, more emphasis be placed on the modelling of basic flows– in this case that of a free jet, for which there is a wealth of high-grade test data available.

Finally, the effect of heat transfer with the walls was only considered by a few participants, and these provided the most accurate results. Although the importance of heat transfer can only be quantified by appropriate parametric studies, it is presumed that it should not be neglected completely for the accurate modelling of the erosion process here considered. This is an example of how the tackling of a new problem might often lead to questionable simplifications and modelling choices.

ACKNOWLEDGMENTS

This benchmark test was carried out by the experimental group of the Laboratory for Thermal-Hydraulics at PSI, composed of G. Mignot, S. Paranjape, D. Paladino, L. Ryan, M. Fehlmann and S. Suter (in addition to one of the authors of this paper, R. Kapulla), The exceptional care they maintained in designing and conducting the experiment, and their personal commitment to produce CFD-grade data to underpin this benchmark exercise is hereby gratefully acknowledged. Thanks are also due to the participants themselves, who performed the blind simulations, and submitted them by the deadline date, to provide the numerical data for the synthesis subsequently undertaken, and reported in this document. We regret that we cannot name them directly and thank them individually, since it was stipulated that complete anonymity of the contributors would be maintained.

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