

## **A BENCHMARK EXERCISE ON THE USE OF CFD CODES FOR CONTAINMENT ISSUES USING BEST PRACTICE GUIDELINES: A COMPUTATIONAL CHALLENGE**

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### **Abstract**

In the framework of the 5<sup>th</sup> EU-FWP project ECORA the capabilities of CFD software packages for simulating flows in the containment of nuclear reactors was evaluated. Four codes were assessed using two basic tests in the PANDA facility addressing the transport of gases in a multi-compartment geometry. The assessment included a first attempt to use Best Practice Guidelines (BPG) to the analysis of long, large-scale, transient problems. Due to the large computational overhead of the analysis, the BPGs could not fully be applied. It was thus concluded that the application of the BPGs to full containment analysis is out of reach with the currently available computer power. On the other hand, CFD codes used with a sufficiently detailed mesh seem to be capable to give reliable answers on issues relevant for containment simulation using standard two-equation turbulence models. Development on turbulence models is constantly ongoing. If it turns out that advanced (and more computationally intensive) turbulence models may not be needed, the use of the BPG for ‘certified’ simulations could become feasible within a relatively short time.

### **Introduction**

The need for more accurate computational methods for the analysis of nuclear reactor systems has produced a growing interest for Computational Fluid Dynamics (CFD) and a constant expansion of the range of applications of CFD codes. In particular, some specific problems arising from the development of advanced LWR has motivated a large research activity for exploring the application of CFD codes to the analysis of containments. However, the use of CFD codes for containment analysis as well as, in general, in nuclear engineering is still hindered by the lack of a systematic assessment of costs and benefits of the use of these methods. Moreover, analyses based on “one shot” calculations (often presented in the technical literature), which are motivated by the high computational costs and

the prescribed time frame of the projects, do not contribute to the trust in CFD methods. To overcome these difficulties, two main issues have to be addressed:

- establishment of quality criteria and evaluation of the costs resulting from their use
- basic validation of codes using high-quality, detailed experimental results

The 5<sup>th</sup> EU-FWP project ECORA [1] has been a first step towards the establishment of commonly accepted quality and performance criteria and the identification of the application areas where the use of CFD tools can lead to accurate results at acceptable costs. One of the most important components of the project was the definition of best practice guidelines (BPG), which define the standards for the assessment of CFD software and results. Among others, they ‘...aim at quantifying and reducing numerical errors so that modeling error can be properly estimated’ [1]. The establishment of BPGs is of paramount importance for building confidence in CFD, as also shown by on-going international activities [2]. An equally important consideration is the evaluation of the impact of these quality criteria on the analysis of specific problems of significance for nuclear safety, as the definition of realistic goals is necessary to avoid the delivery of unacceptably incomplete analyses under the pressure of cost and time requirements.

The second aspect to consider in the qualification of CFD codes for containment application is their basic validation. Although a number of experiments and code validation exercises have been made in the past and new research programmes are currently in progress for the assessment of codes for prototypical conditions (where condensation plays an important role), little evidence exists that the codes can adequately predict in a complex geometry the underlying, basic gas transport processes, which are also controlled by inertia, buoyancy and turbulence effects.

Within this general framework, the analyses presented here aimed at investigating the capabilities of CFD codes to reproduce flows of interest for the containment response to a hypothetical accident and to provide an evaluation of the applicability of the BPGs to these large-scale, transient problems. Therefore, this work addresses the basic capabilities of the codes to predict the flow structures produced by fluid injections in large vessels and the associated gas transport, mixing and stratification in interconnected gas volumes. To this aim, the assessment must use separate-effect test data collected in facilities where the 3-D distribution of the relevant variables is measured with sufficient resolution and accuracy, and tests are performed under well controlled initial and boundary conditions. Tests that have been especially designed to provide the adequate database for this basic assessment are carried out in the PANDA facility [3], within the OECD SETH project [4]. This paper mostly addresses the structure of the benchmark exercise and the computational challenge posed by the problem investigated, whereas limited comparison of the simulations with the experimental results (not discussed here) is only presented to provide a first estimation of the accuracy that can be achieved in the simulation of basic flows with the presently available computer power.

## **Tests chosen for the benchmark**

### ***The PANDA facility***

The PANDA facility, which is shown in Figure 1, is well suited for basic experiments at large scale, in view of its size, the twin-vessel geometry (two couples of vessels connected by large pipes) and its flexibility. For most tests, only the two upper vessels (Drywells) and the large pipe (interconnecting pipe) that connects them are used. Fluid is injected in one vessel (Drywell 1, DW1), and the gas distribution in that vessel, as well as the distribution of gases and the propagation of the stratification front in the adjacent one (Drywell 2, DW2) are measured.

### ***The OECD experimental programme***

The OECD-SETH experimental programme [4] includes various types of tests, where the distribution of gases within the two Drywells is controlled by the horizontal or vertical injections of steam or steam/helium mixtures in one vessel. Most tests are performed with a constant pressure boundary condition, prescribing the pressure at the outlet (vent), and under conditions for which no condensation is expected: a moderately superheated gas is injected in an ambient where both gas and walls are at a temperature slightly above the saturation temperature at the prescribed pressure. The programme includes, however, some tests with condensation (not reported here). Measurements include pressure, injection and vent flow rates, fluid and wall temperatures, gas concentrations, and velocities at selected locations. PIV measurements are also made for specific regions. The typical test duration for all tests is a few thousand seconds, which is a computational challenge for simulations using CFD codes with high-quality meshes. Additional information on the experimental programme, its rationale and the available instrumentation is included in Ref. [5].

### ***Tests selected for the benchmark exercise***

Two tests without condensation (identified by number 9 and 17, respectively) have been selected, which feature low-elevation, horizontal injection of steam close to the wall of one of the two initially air-filled vessels: one with a very low-momentum injection (Test 9, with inlet velocity about 1 m/s) and one with higher (but still low) momentum injection (Test 17, the inlet velocity being about 5 m/s). For both tests, the pressure was maintained constant during the transient as fluid was vented to the atmosphere through a pipe connected to a flange at the top of Drywell 2. The schematics of both tests is also shown in Fig. 1. The two tests lead to different jet penetrations  $s_p$  and flow structures in the fluid receiving vessel. Indeed, Test 17 was expected to result in a highly-buoyant jet, with axis detached from both walls, producing anti-clockwise circulation in Drywell1 in the plane of the jet. Test 9, instead, is expected to result in a near-wall plume and clockwise circulation. This experimental set-up produces a flow condition where the buoyancy force acts perpendicular to the initial inertia of the injected flow, a configuration which has been investigated little in the past and is specially challenging for the codes.

### ***The scoping exercise***

As discussed above, the BPGs should be applied for evaluating the capabilities of the codes. However, due to the large computational overhead that they impose (among others, sensitivity studies with respect to mesh, time step, etc.) the application of BPGs to the analysis of the PANDA SETH tests needed to be evaluated, and realistic goals had to be set. To this aim, a scoping exercise was conducted, which gave the opportunity to gain some familiarity with the typical computation times associated with the simulation of the tests included in the PANDA SETH test matrix on the specific computer platform that has later been used for the benchmark exercise. This preliminary information has been used for the final selection of the tests (injection velocities), as well as for defining the time span of the tests to simulate and a set of recommendations that the participants in the benchmark were expected to apply. Due to the exploratory character of the simulation, the analysis for typical conditions could be limited to a simplified geometry (one vessel and half interconnecting pipe only) and boundary conditions. The exercise proposed, however, was intended to be representative of the real case.

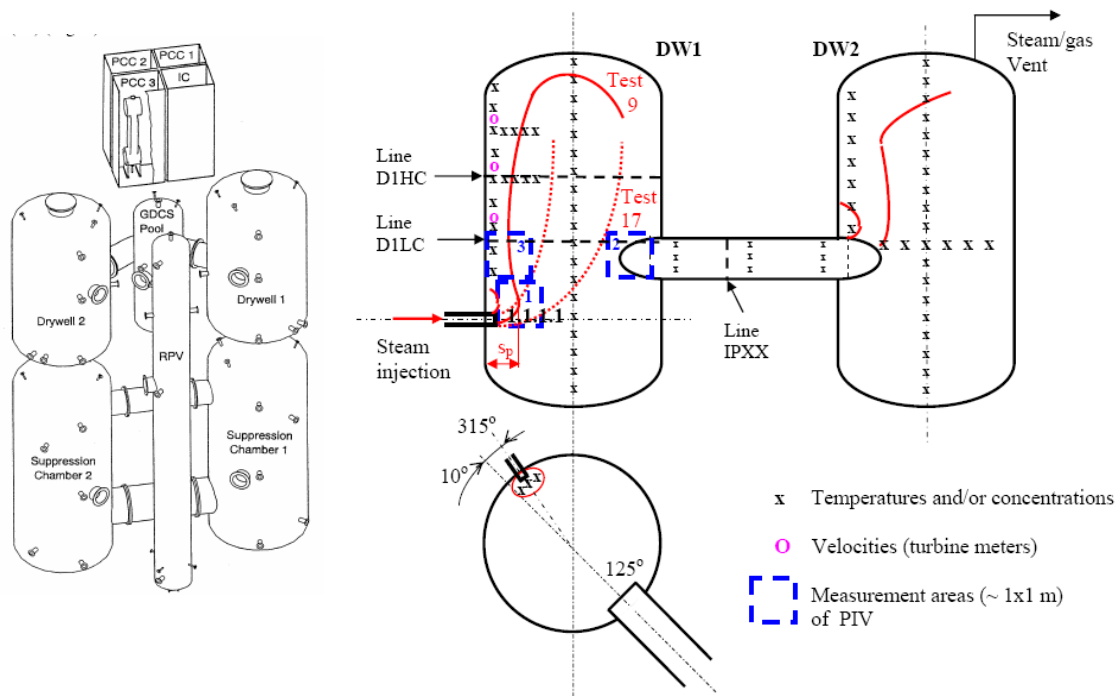


Figure 1: The PANDA facility (left) and configuration for the two PANDA SETH tests selected for the benchmark exercise in the ECORA project (right).

It was thus proposed to study the first period of a representative transient relevant to condition of Test 17 in a “box” geometry, where the volume of the vessel and the most important linear dimensions (hydraulic diameter of the injection pipe, distance of the injection from the opposite wall, height of the connecting pipe, height of the vessel) were maintained. The detailed information on the scoping exercise is included in [5]. The scoping test was calculated by the seven partners in one of the Work-Packages of the ECORA project (PSI, GRS, VTT, Vattenfall, CEA, AEKI and NRI) using three of the four codes that have later been assessed using the SETH data, i.e., CFX-4 [6], FLUENT [7] and TONUS [8]. Additionally, calculations with the GOTHIC code [9] were also carried out, as most of the pre-test calculations for defining the test conditions for the SETH project have been performed using this code. Mesh sensitivity studies were prescribed starting from a basic mesh, using at least one refined mesh.

The results showed that: 1) large computation times were required for the simulation with the refined mesh, and small time steps were necessary for achieving a sufficiently accurate solution; 2) no mesh-independent results could be obtained with the meshes used, and a large sensitivity in the results exists with respect to the mesh used; 3) the turbulence model used substantially affected the results.

### Definition of the benchmark (validation) exercise

It was then concluded that the currently available computer resources are not sufficient for a complete analysis of the entire transient of Tests 9 and 17 using the BPGs. Indeed, simulations of up to a few thousand seconds using increasingly fine meshes to obtain converged solutions appeared not to be possible. Simulations of the entire transients with only one, “practical mesh” seemed to be the only

realistic option. The BPGs could only be applied to a portion of the transient. For a short transient sensitivity studies aiming at evaluating the various errors and the accuracy of the simulation were expected to be possible. Therefore, the validation exercise could be conveniently divided in two steps:

*Step 1:* it was required to perform the simulation according to the BPGs for a short transient: 250 s for Test 9 and 70 s for Test 17, respectively. Since the steam concentration in the interconnecting pipe has a crucial role in the simulation, (it “integrates” the errors in the simulation of the flow and transport processes in the Drywell 1) the end of Step 1 is conveniently defined by the time at which the steam concentration of the air-steam mixture that is flowing through the interconnecting time is sufficiently high to be detected with confidence. This time, evaluated with the GOTHIC code, was estimated to be about 70 s for Test 17 and between 200 s and 250 s for Test 9.

*Step 2:* provided that the solution using a “practical mesh” was sufficiently close to that obtained with the finest mesh used in Step 1, the entire transient had to be calculated with that mesh. The criterion used for deciding whether Step 2 has to be carried out was decided to be the convergence of the target variables (see below) within certain acceptance limits, to be prescribed. It was then agreed, that this simulation had to be performed only if the simulations of Step 1 showed that the calculation of the target variables with the largest “practical” mesh and the finest mesh did not differ by more than 5%. The calculation with the largest “practical” mesh had to be extended to the time when the stratification front in Drywell 2 was expected to propagate below the interconnecting pipe. In the two tests, the time of this event was estimated to be 4000 s for Test 9 and 2000 s for Test 17, respectively. The actual test duration was about 2400 s for Test 17 and 7200 s for test 9.

Specifications for the pre-test analyses were given for: geometry, simulation times, initial and boundary conditions, sensitivity studies, as well as for the variables to submit [5]. The requirement to use second order methods was satisfied with all codes but CFX-4.4, as this code could only run using first order methods due the very small time steps associated with the use of higher-order methods.

The two tests were started from the same initial conditions: pressure at 1.3 bar, wall and fluid temperature at 108 °C, the two vessels filled with air at zero velocity conditions. Superheated steam at constant temperature (140 °C) was injected at about 1 m/s in Test 9 and at about 5 m/s in Test 17, respectively.

### ***Sensitivity studies required according to BPGs***

*Assessment of the numerical error.* The strict application of the BPGs would result in a computational effort that is hardly affordable with the current computer power. Especially a systematic refinement of the mesh (at least in two steps), which would allow the formal definition of the discretisation error, could not be required, as it would have led (starting from a coarse mesh of about  $10^5$  cells and halving twice each cell in all three directions x, y and z) to a fine mesh of several million cells. It was therefore recommended to refine the mesh according to the experience of the user, and to evaluate the convergence of the simulations using the trends of the target variables. It was therefore excluded that the same mesh could be used by all participants in the validation exercise, or strict criteria could be prescribed for establishing the mesh. Also, the guideline to verify that the results obtained are independent of the prescribed accuracy (time step or tolerance on residuals) was somewhat relaxed, and such independence was required to be verified for one mesh only. As regards the truncation error, experience shows that it may not be always possible to get converged solutions at both single and double precision. Therefore, the investigation on the effect of the precision on the results was suggested only. In summary, it was required to perform the following sensitivity studies: 1) use three meshes (coarse, intermediate, fine); 2) study the effect of time step (tolerance on residuals)

for at least one mesh (intermediate mesh), using at least three time steps; 3) If applicable, study the effect of precision.

*Assessment of the modelling error.* The only model that was expected to have an effect on the calculated results is the turbulence model (and, to some extent, the associated wall treatment). This implies that the validation exercise should include simulations with at least two turbulence models. The requirement of the BPGs to include in the sensitivity study a substantially different turbulence model (e.g., RSM) could not be considered for this exercise. As the standard high-Reynolds number  $k-\varepsilon$  model is currently the industrial standard for large-scale calculations, all participants were asked to provide simulations with this model. The criteria defined in the BPGs regarding the appropriate wall treatment for the various turbulence models and the associated requirements for the mesh close to the walls had to be applied.

Target variables were defined for Step 1 only, as sensitivity studies were only requested for the early time period. These were the steam molar fractions on a horizontal line in DW1 and a vertical line in the middle section of the interconnecting pipe (indicated in Fig. 1). The specified horizontal line was aligned with the axis of the injection and was at different elevations for the two tests (D1HC and D1LC for Tests 9 and 17, respectively). The convergence of the simulation was estimated by calculating the normalized RMS of the differences of the distributions along those lines obtained with the increasingly fine meshes:

$$RMS \text{ difference} = \frac{1}{|f_{1,max} - f_{1,min}|} \sqrt{\frac{\sum_{i=1}^N (f_1 - f_2)^2}{N}}$$

where  $f_1$  and  $f_2$  are the values of the variables (temperatures or concentrations) at  $N$  points for the calculations with two different meshes, respectively, for each prescribed line. The target variables were used for evaluating the convergence of the simulation, and did not all correspond to variables actually measured in the test.

## Main results of the pre-test analyses

Simulations have been submitted with 4 codes: CFX-4, CFX-5 [10], FLUENT and TONUS. The pre-test calculations revealed that the application of the BPGs (though reduced in scope) to the analyses of the transient problem in the large-scale geometry of the PANDA facility resulted in a severe computational challenge. Therefore, an overview of the simulations performed and the statistics of the simulation is presented first.

### Overview of simulations performed

Most of the organisations could not perform all the sensitivity studies prescribed, and none of the results delivered can be considered fully converged in the sense of the BPGs. Tables I, II and III present a few essential aspects of the calculations performed (not all calculations are listed in these tables). A more comprehensive summary of the analyses carried-out is presented in [11].

A first, general observation is that the number of cells used for most calculation is in the range a few hundred thousand cells to one million. The level of detail of the mesh used is partly a consequence of two specific features of the PANDA facility: 1) Small vent pipe, which forces small cells close to the vent and consequent propagation of a fine mesh in regions of flow where detail is likely not to be required (this problem is obviously more severe for structured meshes); 2) presence of pipe

protrusions. Although this latter detail of the geometry is likely not to play an important role in the gas transport, its effect cannot be ruled out “*a priori*”. Therefore, in accordance with the BPGs, the recommendation was made to include these details in the geometrical model.

However, the details do not substantially affect the mesh required. In fact, in view of the difficulty to achieve converged results in the scoping exercise (with a simplified geometry), it can be assumed that the mesh needed for the appropriate representation of the flow in the vessels (ignoring geometrical details) cannot be much smaller than that used for the complete simulation discussed here. This consideration also implies that CFD simulation of gas transport phenomena in a large-scale, multi-compartment geometry of the size of PANDA is likely to require the same detail as that used for the present demonstration case. A second, general remark is that both test cases have posed a severe computational challenge. It can be observed that even for the short period simulations (70 s for Test 17 and 250 s for Test 9), the running time (or CPU time, the information collected being somewhat non-homogeneous) is in the range of several days to a few weeks per run, using state-of-the-art, single-processor computers or, for codes that can be run in parallel mode, small clusters. This large computational overhead strongly limited the scope of the analyses for most organisations, and prevented a systematic application of the BPGs.

Nevertheless, a number of interesting comparisons could be produced and definite conclusions could be drawn, so that the global aim of the exercise could be achieved (see next sections).

Table I: Summary of simulations for Step 1 of Test 9 (250 s transient)

Organisation	Code	Mesh (thousands of cells)	Turbulence model *	Sensitivity to time step	RMS of target variables (D1HC, IPXX) at 250 s **	Hours computation time (Number processors)
AEKI	FLUENT 6.1.22	530	k-ε	no	0.57, 0.53	
		745				1248 (1)
GRS	CFX-5.7	147	k-ε	yes	0.04, 0.24	51 (6)
		335				
		817				
		335	SST	no		60 (6)
PSI	CFX-4.4	300	k-ε	no	0.115, 0.03	168 (1)
		700	RNG			264 (1)
		300			0.07, 0.06	312 (1)
		700	288 (1)			
VTT (DW1 only)	FLUENT 6.1.22	16	k-ε	no	0.09, 0.38	
		33				
		52				90 (1)

Table II: Summary of simulations for Step 1 of Test 17 (70 s transient)

Organisation	Code	Mesh (thousands of cells)	Turbulence model *	Sensitivity to time step	RMS of target variables (D1LC, IPXX) at 70 s **	Hours computation time (number processors)
CEA	TONUS V2004	75	Mixing Length (MixL)			28 (1)
		93		yes	0.03, 0.065	38 (1)
		184			0.14, 0.139	188 (1)
GRS	CFX-5.7	147	k- $\epsilon$			
		335		yes	0.07, 0.12	35 (6)
		799			0.19, 0.05	61 (6)
		335	SST	no		36 (6)
NRI	FLUENT 6.1.22	235	k- $\epsilon$			55 (2)
		480		yes	0.2, 0.11	90 (2)
		890			0.077, 0.025	250 (2)
		480	RNG			100 (2)
		480	Realizable			200 (2)
PSI	CFX-4.4	300	k- $\epsilon$			302 (1)
		700		10 s only	0.09, 0.07	785 (1)
		1100			0.06, 0.03	1224 (1)
		700 ***			0.11, 0.07	400 (1)
		700	RNG			744 (1)
VATTENFALL	FLUENT 6.1.18	45	k- $\epsilon$			48 (4)
		45	RNG	Sensitivity to convergen ce criterion	0.4, 0.07	48 (4)
		363				192 (4)

Table III: Summary of simulations for Step 2 of Tests 9 and 17

Organisation	Code	Mesh (thousands of cells)	Turbulence model *	Transient time	Hours computation time (number processors)
<b>Test 9</b>					
AEKI	FLUENT 6.1.22	745	k- $\epsilon$	450	528 (1)
GRS	CFX-5.7	335	SST	4000	351 (10)
<b>Test 17</b>					
CEA	TONUS V2004	93	Mixing Length (MixL)	2000	300 (1)
GRS	CFX-5.7	335	SST	2000	245 (12)
NRI	FLUENT 6.1.22	480	k- $\epsilon$	2000	1000 (2)

\* For a short explanation, see footnote at pag. 10.

\*\* RMS of the difference between distributions obtained with a mesh and the coarser one. If three meshes have been used, two values are thus given. NRI used a different definition of the RMS, which resulted in lower values.

\*\*\* The only calculation with CFX4.4 using second order methods. The RMS is calculated for the solutions with the 700K mesh using first and second order methods, respectively. It shows that the solution is not converged.



Analysing in more detail the Tables below, a number of observations can be made. In many cases, the matrix of calculations is not complete not only because of the large computation times, but also because of numerical difficulties appearing during the simulation, that forced the transient time to be reduced or termination of the simulation [11].

As stated above, none of the organisations could provide a “certified” simulation of the first period (step 1) in the sense of the BPGs. In fact, all analyses failed to achieve a mesh- and time step-independent solution: either the sensitivity studies could not be made for the problems above, or the RMS of the target variables was higher than the stipulated tolerance (5%). The set of simulations of NRI is the most complete and the closest to the target, so that the intermediate mesh (used for step 2) can be considered approximately “certified”. However, also this analysis is at variance with the strict application of the BPGs in relation to the refinement of the mesh. In fact, the ratio between the coarsest and the finest mesh used is 4 only, instead of 64, which would result from twice halving the size of the cell lengths in all directions.

In summary, the pre-test analysis of the two PANDA tests revealed that the accurate simulation of the transport of gases in a complex geometry for the conditions studied in the first two tests (horizontal injection) is a computationally challenging task that cannot be fully tackled (in the sense of the BPGs) with the presently available computing power.

## Comparison of results

In this section, the main results of the simulations submitted will be presented. Due to confidentiality, experimental results cannot be displayed in a quantitative form, and only essential information is used in the present discussion. More details on Test 17 are given in [11], which has however, limited distribution. The main features of the facility and of the instrumentation used for the experimental programme, as well as some aspects of Tests 9 and 17 are presented in [12,13]. For the sake of the present discussion, it is sufficient to say that the specifications for initial and boundary conditions were matched in both tests and accurate data could be collected. It should be mentioned here that for Test 17 four repeat tests have been performed, with good repeatability, as discussed in [13].

The analysis of the results refers to the three main aspects of the transients investigated, namely flow structure in DW1, steam transport from DW1 to DW2 and to the vent, and stratification in both vessels. In the following presentation, temperature measurements will only be used for identification of the flow structure in the fluid-receiving vessel, and mostly the experimental and calculated concentrations are presented and discussed. The reason is that all simulations (also with other codes not included in this exercise) predict too high temperatures, probably because of the incapability to correctly predict large heat transfer rates with the walls. This aspect of the simulations will not be addressed here.

As a number of sensitivity studies have been made with respect to mesh, time step, etc., it would not be practical to include in the comparison the results of all calculations. Therefore, for each turbulence model used, only the results of the “trust worthiest” calculation (that which is supposed to be affected by the smallest numerical error) were included in the comparison plots.<sup>1</sup> The initial intention was to include in the comparison only “numerical-error-free” simulations, in order to

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<sup>1</sup> The labels in the comparison plots include the name of the organisation, the code used, the number of cells (in thousands) in the mesh, and the turbulence model used (where MixL=Mixing Length; k-ε=standard k-ε model; RNG, Realizable=other variants of the k-ε model; SST=variant of the k-ω model).

estimate the model error, but, due to the problems discussed above, the comparison will include simulations affected by both numerical and model error. However it was possible to arrive at some very interesting conclusions. Simulations for Step 1 have been provided by all partners in the project.

For Step 2, however, fewer contributions were submitted, due to the very large computation times and/or to the failure to obtain converged results (within 5% for the target variables, see Tables I and II) for Step 1.

### Test 9

*Flow structure in the fluid-receiving vessel (Drywell 1).* The flow structure in Drywell1 can be characterised using the experimental information obtained from the arrays of thermocouples placed along horizontal lines. In fact, the peak in the temperature distribution indicates the position of the axis of the plume. Figure 2 shows the temperature distribution along the diametral line D1LC (see Fig. 1) at 250 s (end of Step 1). The low-momentum injection is calculated to produce a plume with axis close to the wall, which persists through the 4000 s transient. Five out of six calculations predicted the axis of the plume to be at about 0.5 m from the wall, which correspondsto the observed displacement of the plume from the wall (the plume being approximately centered with respect to the axis, see [12]).

The large overprediction of the temperatures is reckoned to be mostly due, as already mentioned above, to the strongly underpredicted heat transfer with the wall. The comparison (not shown) of simulations with concentration measurements at two locations in the plume shows, however, that the trajectory of the plume, as well as its horizontal spreading with distance from the injection, must have been well predicted.

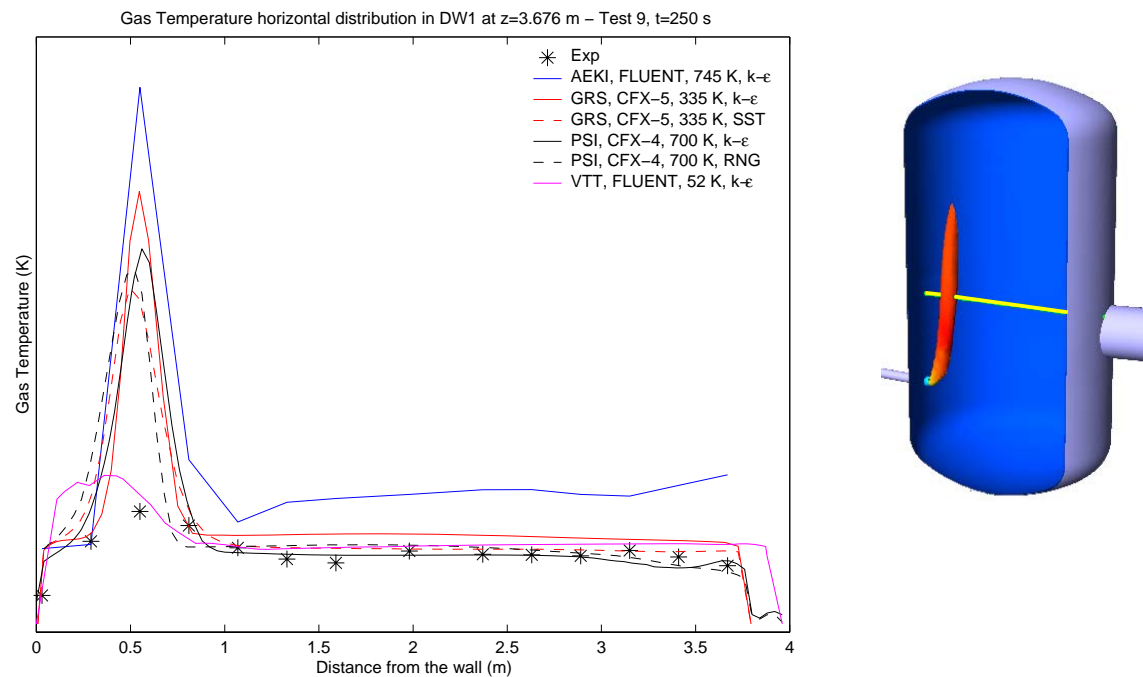


Figure 2: Test 9. Steam temperature distribution at 250 s (end of step 1) along a horizontal line crossing the plume.

The only simulation (from VTT) that shows low temperatures and a maximum closer to the wall has a maximum of the steam concentration (not shown) close to the wall and predicts a larger vertical dilution of the steam concentration: it is thus probably affected by a large numerical error, as the coarse mesh used is likely not to be adequate to resolve the details of the flow and to account for the effects of inertia and buoyancy forces immediately downstream of the injection. Therefore, in the following discussion the calculation with the coarse mesh will not be considered. The important result that it has delivered, however, is that a mesh of less than 100'000 cells for the fluid-receiving vessel (although this hybrid mesh featured a higher concentration of nodes in the regions where higher gradients of the variables were expected) is not sufficiently fine to capture the flow structure for the low momentum injection of Test 9.

*Steam transport through the interconnecting pipe and to the vent.* The substantial agreement of all fine-mesh calculations with respect to the flow structure also results in a good agreement in relation to the inter-compartment steam transport. As the measurement of the steam vertical distribution is not available in the early stage of the transient, only the results obtained for Step 2 (from 250 s) are compared with data. Figure 3 shows the results of the only simulation (with an “uncertified” mesh) carried out for the entire transient at various times: good agreement is observed nearly to the end of the simulated transient. The steam concentration at the vent exit was also well predicted, as shown in Fig. 3.

*Stratification in DW1 and DW2* In accordance with the horizontal distributions, also the distributions along vertical lines at early times predicted by the various fine-mesh calculations were nearly identical, with no penetration of steam below the level of the injection before 250 s. Figure 4 shows the (long-term) evolution in time of the steam molar fraction vertical distribution in the fluid-receiving vessel calculated with two codes. A small difference can be observed between the results provided by AEKI (with FLUENT and the standard k- $\epsilon$  model) and GRS (with CFX-5 and the SST variant of the k- $\omega$  model) at 400 s, both predicting the stratification front around the elevation of the injection pipe. Later in the transient, the simulation by GRS shows a very slow penetration below the inlet pipe, which is confirmed by the experimental data. Figure 4 also shows the evolution in time of the steam molar fraction vertical distribution in the adjacent vessel. Similarly to the results for DW1, a small difference can be observed between the results provided by AEKI (with the standard k- $\epsilon$

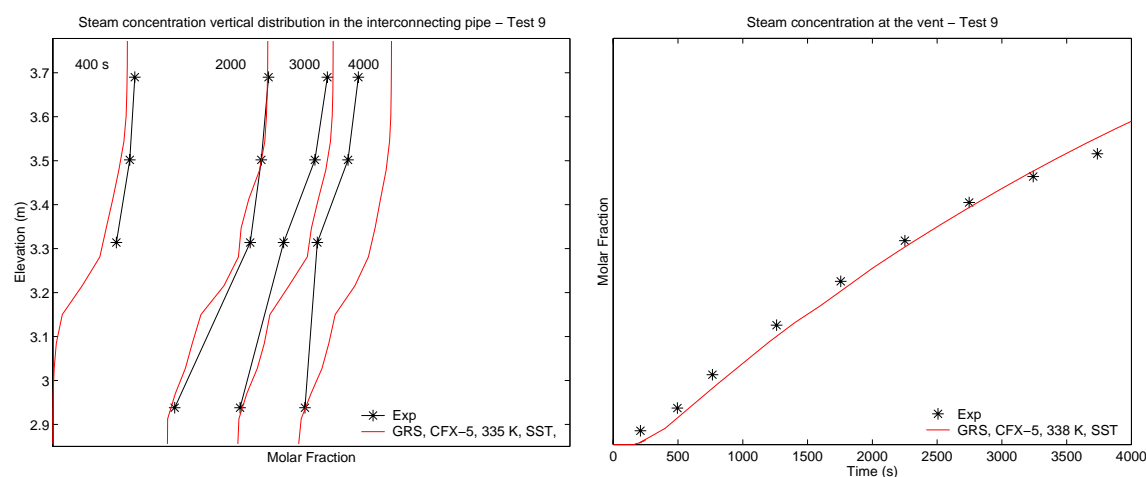


Figure 3: Test 9. Steam concentration vertical distribution in the interconnecting pipe (left) and steam concentration time-history at the vent exit (right).

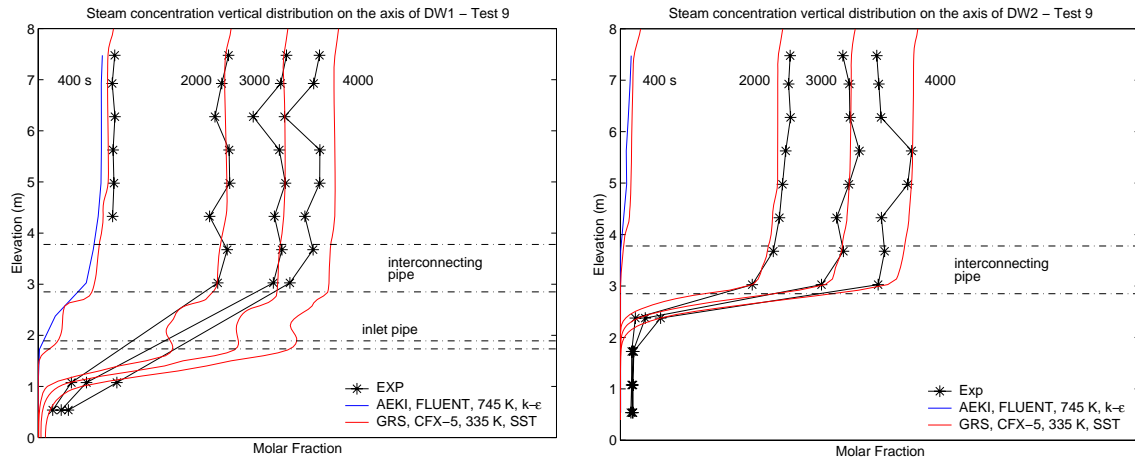


Figure 4: Test 9: Steam concentration vertical distribution in DW1 (left) and DW2 (right) at various times.

model) and GRS (with the SST variant) at 400 s, both predicting the stratification front at an elevation close to the top of the interconnecting pipe. Later in the transient, the simulation by GRS shows a very slow penetration below the interconnecting pipe, which is confirmed by the data.

In summary, it can be observed that a fine-mesh representation of both vessels resulted in good predictions with respect to flow structures and transport processes, independently of the details of the specific geometric models and other assumptions used.

### Test 17

*Flow structure in the fluid-receiving vessel (Drywell 1).* The data show initially a bent jet, which is detached from the wall closer to the injection, but which re-attaches to the wall opposite to the injection point, above the elevation of the interconnecting pipe. In fact, as shown in Figure 5, the maximum temperature along line D1LC is further from the injection than the axis of the vessel (to the “right” of the axis). The observation of the full temperature field in the cross-section at that elevation also shows that the plume is not strictly symmetric with respect to the injection but tends to move towards the interconnecting pipe. Although the position of the maximum is fluctuating, it initially remains at a distance between 2 m and 2.5 m from the wall of the injection. Later in the transient, the jet loses buoyancy and the axis of the jet becomes increasingly horizontal, and at the end of the transient it nearly enters the interconnecting pipe directly. The slow variation of the inclination of the initially buoyant jet was also confirmed by the PIV observations. The relatively large horizontal penetration of the jet results in an anti-clockwise circulation all over the transient, as expected.

Figure 5 shows that the calculated results are in a broad band, the predictions indicating a temperature peak between 1.3 m and 2.5 m from the wall. All calculations using two-equation models qualitatively predict the large penetration depth of the jet, although the results span over more than half a metre. The best agreement was obtained by NRI with the FLUENT code and a rather fine mesh. All these calculations correctly predict anti-clockwise circulation. However, the only calculation with the Mixing Length turbulence model produces a much less inclined flow, resulting in clockwise

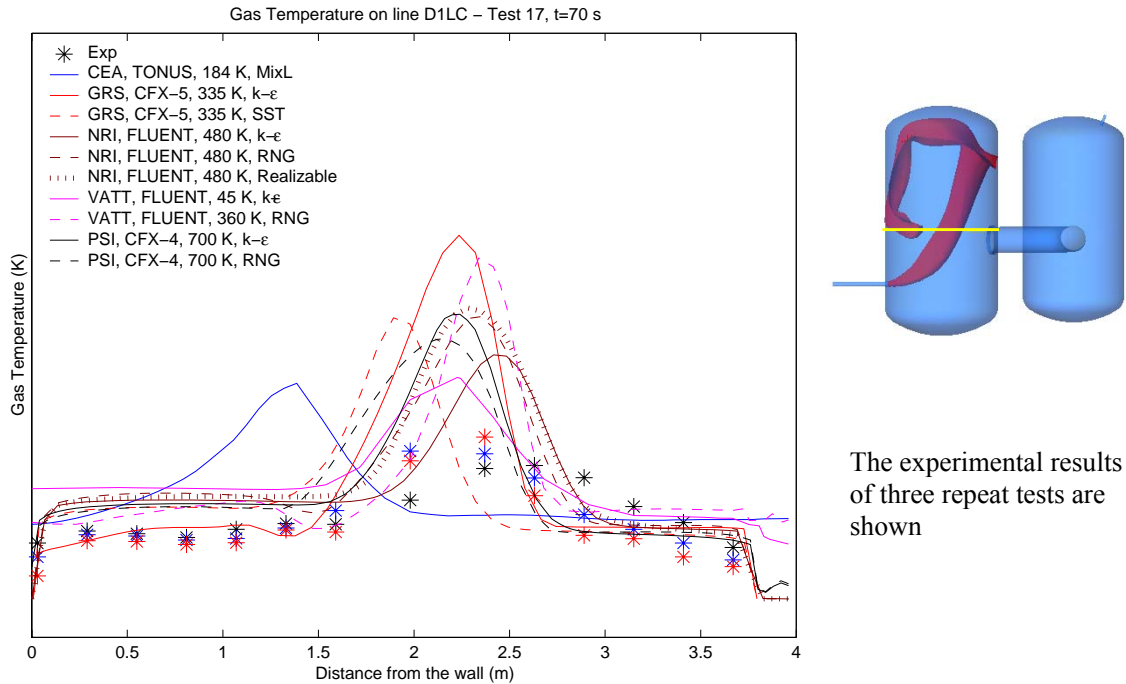


Figure 5: Test 17. Gas temperature distribution at 70 s (end of step 1) on a horizontal line crossing the jet.

circulation. The predicted temperatures are in all cases higher than the experimental ones, and the width of the jet was underpredicted in all simulations, for reasons that are difficult to identify. The temperature profiles are thus to be regarded as an indication of the position of the buoyant jet only. With respect to this aspect of the test, it can be concluded that some of the CFD predictions were very successful.

The rather large spread in the results is partly justified by certain assumptions made on the inlet conditions and the flow development inside the inlet pipe. However, the large differences between calculations in relation to the spatial evolution of the jet are mostly due to the effect of the mesh and the model used. This observation shows the importance of arriving at mesh-insensitive results before studying the effect of the various physical models. In particular, only the results obtained by NRI can be used for judging the merits of the three models investigated. For all other organisations, the differences between predictions are likely to be affected by both mesh and model effects.

*Steam transport through the interconnecting pipe and to the vent.* Figure 6 shows, the vertical distribution of steam in the interconnecting pipe at two times. It can be observed that the predictions using the  $k-\epsilon$  model are nearly overlapping the experimental results at 500 s. This agreement, although somewhat less impressive, is preserved at later times.

On the other hand, the calculation with the Mixing Length model overpredicts the total amount of steam transported through the interconnecting pipe. The difference between the results obtained with the two models is likely to be associated with the difference in the predicted flow structure in DW1, the clockwise circulation predicted by TONUS resulting in an earlier and larger penetration of a steam-rich mixture into the interconnecting pipe. The differences in the steam transport through the interconnecting pipe are reflected in similar differences in the steam concentration at the vent (top of

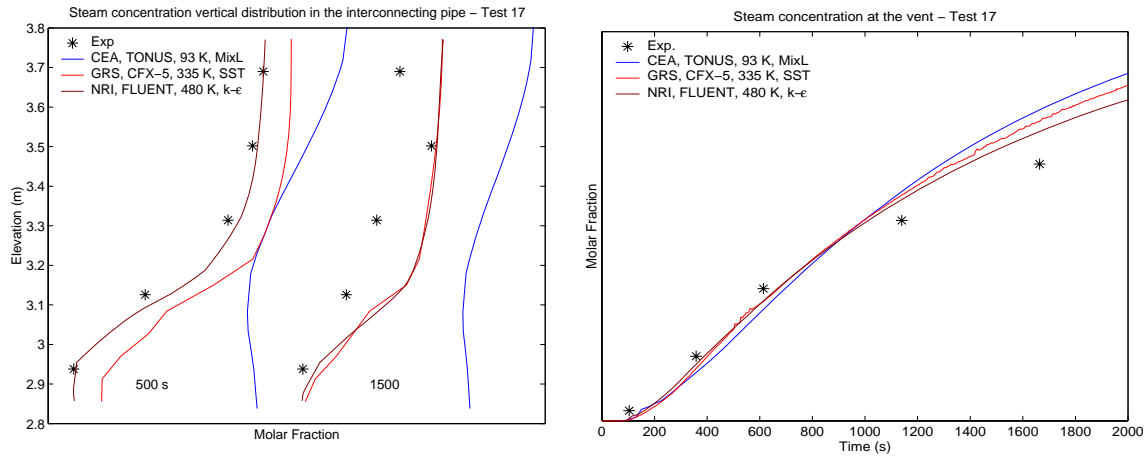


Figure 6: Test 17. Steam concentration vertical distribution in the interconnecting pipe at two times and steam concentration time-history at the vent exit.

DW2). In fact, Figure 6 shows that all codes predict the steam molar fraction at the vent pipe inlet pretty well, and the predictions closest to the test data are those obtained with the FLUENT code, whereas the largest deviation is observed in the predictions with TONUS (using the Mixing Length model).

*Stratification in DW1 and DW2.* Figure 7 presents the comparison between calculated and measured concentrations in both Drywells at 1000 s. It is easily realised that the predictions for DW1 using two-equation models are in excellent agreement with the data. In particular, the distinct steam concentration peak at an elevation slightly above the injection level is well captured by both CFX-5 and FLUENT (using variants of the  $k-\omega$  and  $k-\epsilon$  model, respectively), which indicates that the flow structure at this late stage of the transient is well predicted. Moreover, the persistence of a steam-lean region in the lower head of the vessel is predicted very well by CFX-5 and fairly well by FLUENT.

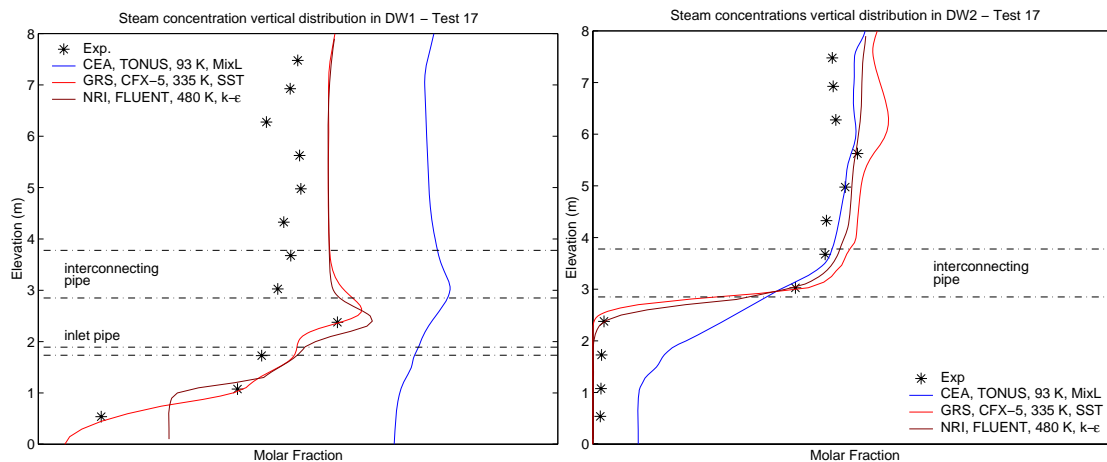


Figure 7: Test 17. Steam concentration vertical distribution in DW1 and DW2 at 1000 s.

In contrast, the large diffusivity associated with the Mixing Length model causes TONUS to predict a concentration profile much flatter than in the experiment (the larger concentrations at all elevations along the specific vertical line are probably due to 3-D effects). Figure 7 also shows the steam concentrations in DW2 measured at 1000 s. Again the predictions with the codes using two-equation models are in excellent agreement with the data, the sharp stratification front below the interconnecting pipe being reproduced very well. It is worth remarking that rather large differences in the flow structure predictions in the fluid-receiving vessel (see above) resulted in a minor difference in the steam distribution in the adjacent vessel. However, TONUS overpredicts the thickness of the interface between the steam-rich upper part of the vessel and the steam-lean bottom part, as a consequence of the large diffusivity calculated with the Mixing Length model.

In summary, the pre-test analyses of Test 17 revealed that the prediction of the flow structure in the fluid-receiving vessel is very sensitive to the mesh and the model used. Moreover, simulations approaching the numerical-error-free condition show that the standard k- $\epsilon$  model is the most appropriate for reproducing the special flow conditions (horizontal injection and moderate velocity) investigated here. As for stratification and gas transport over long times, the details of the model and the mesh seem to matter less, and very good predictions could be obtained with both CFX-5 and FLUENT using two-equation models. On the other hand, the use of the Mixing Length model led to somewhat less accurate results.

## Conclusions

In the ECORA project the need for a basic assessment of CFD codes for flows relevant for containment analysis has been addressed, using the first results of an experimental programme (OECD SETH) specially conceived for this purpose. Certain conclusions (especially those related to the physical models used) are preliminary, and need to be verified for the conditions specified for the other tests in the SETH programme. Various results of the exercise (especially those related to the applicability of the BPGs), however, can be used for evaluating the perspective use of CFD for the analysis of reactor containment. The main outcomes of the work performed are:

- The accurate analysis of the flows produced by the injection of buoyant fluid via small pipes into large-size, interconnected vessels is a computationally challenging task, which requires very large computer resources. For the conditions investigated here, several hundred thousand cells were required for obtaining sufficiently accurate results. The need for such a large mesh, together with the long times of the transients investigated, result in very large computation times.
- Due to the large computational overhead of the analysis, the BPGs had to be reduced in scope. In particular, it was decided to use the BPGs for an initial phase of the transient, and to use the mesh thus “certified” also for the long-term calculation. This approach, obviously, can only be proposed for transients where boundary conditions and the main variables are expected to change monotonically and slowly (as, for instance, in the case of a continuous build-up of a gas). Notwithstanding the reduced scope, the BPGs could not fully be applied by any organization involved in the benchmarking exercise. In a strict sense, simulations using a mesh with about  $10^6$  cells were not proved to have achieved mesh-insensitivity.
- The success of the simulation (against experimental data) performed with an approximately “certified” mesh seems to confirm that the application of a systematic sensitivity study (along the lines of the BPGs) has a high “pay-off”. On the other hand, the adequate predictions obtained with a mesh of similar size, but not supported by sensitivity studies and evaluation

of the accuracy, could lead to the erroneous expectation that the use of a “good” mesh according to engineering judgement and careful choice of numerical methods and time step could be sufficient to produce a trustworthy result. This success of the “traditional approach” should not distract attention from the need to establish rigorous guidelines.

- The use of two-equation models for turbulence produced unexpectedly good results. On the other hand, the simpler Mixing Length model produced results of much less accuracy in relation to all aspects of the transient, the flow structure in the fluid-receiving vessel being totally missed. The flows analysed here do not include all the physics (principally condensation is not included) of prototypical applications. However, the success obtained in the simulation of the separate-effect tests considered here using appropriate mesh and models can greatly improve the confidence in the methods used generally for containment analysis.

In relation to the objective of this work in the more general framework of the ECORA project, namely the evaluation of CFD methods for reactor safety analysis, the following conclusions can be drawn:

- The applications of the BPGs to full containment analysis is out of reach with the currently available computer power, although the use of large computer clusters (provided that the code is written for parallel computing) could permit occasionally full-scope analyses of reference scenarios.
- In general, CFD codes seem to be capable of producing reliable answers on issues relevant to containment integrity evaluation (such as inter-compartment mass transport, which is the only relevant issue investigated here) using standard turbulence models. Development on turbulence models is constantly ongoing. If it turns out that advanced (and more computationally intensive) turbulence models may not be needed, the use of the BPG for ‘certified’ simulations could become feasible within a relatively short time.
- It would be interesting to repeat this exercise in a few year’s time, to re-evaluate the feasibility of “certified” simulations.

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