Analysis of the influence of the heat transfer phenomena on the late phase of the ThAI Iod-12 test

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Abstract. Iodine is one of the major contributors to the source term during a severe accident in a Nuclear Power Plant for its volatility and high radiological consequences. Therefore, large efforts have been made to describe the Iodine behaviour during an accident, especially in the containment system. Due to the lack of experimental data, in the last years many attempts were carried out to fill the gaps on the knowledge of Iodine behaviour. In this framework, two tests (ThAI Iod-11 and Iod-12) were carried out inside a multi-compartment steel vessel. A quite complex transient characterizes these two tests; therefore they are also suitable for thermal-hydraulic benchmarks. The two tests were originally released for a benchmark exercise during the SARNET2 EU Project. At the end of this benchmark a report covering the main findings was issued, stating that the common codes employed in SA studies were able to simulate the tests but with large discrepancies. The present work is then related to the application of the new versions of ASTEC and MELCOR codes with the aim of carry out a new code-to-code comparison vs. ThAI Iod-12 experimental data, focusing on the influence of the heat exchanges with the outer environment, which seems to be one of the most challenging issues to cope with.

1. Introduction
During the last years many researches were carried out [1] to investigate aerosol behaviour during a severe accident (SA) in a Nuclear Power Plant (NPP). In particular these tests investigated the nuclear aerosol formation, transport and interaction with the various containment surfaces. Moreover, also their influence on thermal-hydraulics of primary circuit and containment system has been investigated [2]. A quite large part of these tests focused on the Iodine, being one of the major contributors to the external source term during a SA for its volatility and high radiological consequences [3].

As part of these efforts, the ThAI Iod-12 test [4] was performed. The test treats mainly the Iodine transport, deposition and resuspension from steel surfaces. The test is characterized by an Iodine release in a large steel-vessel under stratified conditions. Following, an helium injection breaks these stratified conditions leading to a mixing atmosphere and then to a mixed atmosphere. Therefore, thanks to the particular thermal-hydraulics conditions achieved during the transient, this test can also be used as thermal-hydraulics benchmark.

ThAI Iod-12 was originally released as a numerical benchmark [4] under the SARNET2 framework [5] in order to investigate the coupling between containment thermal-hydraulic and iodine codes, and to evaluate the capability of the SA codes to simulate the Iodine-steel interactions. At the end of the
benchmark (2012) a report covering the main findings was issued [6], stating that the employed codes, common used in SA studies, were able to simulate the test but large discrepancies were also present, especially on thermal-hydraulics and in Iodine modelling. For these causes model improvements and then further investigations were suggested.

Two of the main SA codes employed in the SARNET-2 framework were ASTEC and MELCOR [7]. Both codes have shown large thermal-hydraulics discrepancies during the benchmark, therefore the scope of this work is to build a new nodalisation capable to correctly simulate the entire thermal-hydraulics ThAI-12 transient and then utilize it with the latest ASTEC and MELCOR code versions. In particular the heat transfer phenomena towards the outer environment is of main concern, for its influence on the local atmospheric temperatures, and thus on the local relative humidity (r.h.). Both the local atmospheric temperatures and the local relative humidity influence the Iodine behaviour, therefore a proper thermal-hydraulics prediction is needed also for a correct evaluation of the Iodine behaviour.

The present article is structured into four parts. The first part describes the ThAI facility and the Iod-12 test. The second one describes the proposed common nodalisation. The third one describes the main thermal-hydraulics results, and finally in the fourth part of the paper the results of the study are reported.

2. The ThAI facility

The ThAI facility, acronym for Thermal-hydraulic Hydrogen, Aerosol and Iodine, is an experimental facility located at Eschborn (D). It is a coupled-effects test facility, simultaneously investigating stratification, convection and wall condensation as well heat conduction and storage in structures. Tests performed are mainly transients governed by the thermal inertia of the containment vessel. The facility is also characterized by a wide and complex instrumentation, allowing the determination of the thermal-hydraulic conditions inside each compartment. Thanks to its characteristics ThAI can be considered as an intermediate step between a separate-effect facility and a prototypical one.

3. Vessel description

The main ThAI component is a cylindrical steel vessel (Figure 1) with a total free volume of 60 m³ (height: 9.2 m, Maximum diameter: 3.2 m). The vessel could resist to pressures and temperatures up to 14 bar and 180 °C and its free volume can be subdivided into six zones: the sump (1.7 m³), the bottom area (6.6 m³), the lower and the upper annulus (11.4 m³ and 15.4 m³ respectively), the dome area (17.7 m³) and the inner cylinder area (6.05 m³).

The lower and upper vessel surfaces are composed by 3 cm of AISI 316 Ti, 12 cm of mineral wool and 1 mm of Aluminum, except the vessel lid which is made in St-35 steel instead of AISI 316 Ti (mineral wool and aluminum thicknesses remain the same). The thermal insulation in the sump and dome areas is ~0.14 W/m·K The external cylindrical vessel surface is composed by three heating/cooling jackets (h/c jackets) characterized by an oil moving helicoidally around the vessel circumference. The h/c jackets are composed (from the inner side to the outer side) by ~2.2 cm of AISI 316 Ti, a gap of ~1.7 cm for the carrier oil, 6 mm of AISI 316 Ti, 12 cm of mineral wool and 1 mm of Aluminium. The thermal insulation for the vertical walls is 0.1 W/m·K and the thermal conductivity of the carrier oil is 1.0 W/m·K. An electrical heater can also provide heat to the sump water.

As addendum, three intermediate decks of AISI 316 Ti were installed inside the vessel to enhance its spatial subdivision during the test. The upper deck closes the inner cylinder at top and reduces the flow area from the upper annulus to the dome area, leaving opened two sections of 0.123 m². The intermediate deck reduces the flow area between the upper and the lower annulus, leaving two sections of 0.198 m² and 0.325 m². The lower deck reduces the flow area from the lower vessel zone to the inner cylinder leaving a section of 0.176 m². Other important vessel components are the condensate collectors dividing the lower and the upper annulus, and the condensate gutters that drain condensate water out of the vessel.
4. The Iod-12 test

The Iod-12 test is characterized by injections of Iodine, Helium and steam as well as of energy by the external h/c jackets and the sump electrical heater. The test can be subdivided into eight phases, but only 6 were simulated, as requested in the SARNET2 benchmark specification [4]. In table 1 the main events occurring during the transient are reported.

Figure 1. Position of the main vessel fittings and sensors.
Table 1. Main events occurring during the Iod-12 test.

| Time       | Event                                                                 |
|------------|-----------------------------------------------------------------------|
| -1.0 h     | Start of the simulation                                               |
| -0.32 h to -0.23 h | Injection of 0.335 Nm³ of helium                                       |
| 0.0 h to 0.1 h | First Iodine injection in the dome area (h = 8.4 m) with air as carrier gas |
| 0.17 h to 0.21 h | Second Iodine injection (same location and carrier gas)               |
| 1.75 h     | Upper and middle h/c jackets switched off.                             |
| 2.62 h to 9.63 h | Injection of saturated steam (109 °C) in the upper zone of the inner cylinder area at a rate of 30 g/s, and then following increased to 34 g/s (4.0 h) and decreased to 4.3 g/s (4.82 h - 5.75 h). Furthermore the steam injection is re-increased to 6 g/s (6.95 h) and ended at 9.63 h. |
| 2.68 h     | Middle and lower h/c jackets switched on full cooling.                |
| 3.7 h      | Activation of the sump electrical heater. Initially at 13.4 kW and then reduced to 3 kW (5.7 h). |
| 4.92 h to 5.22 h | Injection of 563 g of Helium in the bottom area.                     |
| 5.48 h     | Upper h/c jacket switched on.                                         |
| 9.67 h     | Deactivation of the sump electrical heater.                           |
| 9.68 h     | H/c jackets thermal oil circuit switched off, but a limited cooling effect is presents due to the thermal oil natural circulation. |
| 24.4 h to 30 h | Upper h/c jacket switched on full heating initially at 39 kW and then reduced to 3 kW at 25.68 h. |

5. Common nodalisation

The ThAI facility has been modelled (figure 2) employing 66 control volumes, 60 for the vessel (3 volumes for the sump zone, 6 in the bottom area, 8 for the lower annulus, 16 volumes for the upper annulus, 14 in the dome area and 13 for the inner cylinder), 5 for the drain discharge volumes and 1 simulating the outer environment. The dome is vertically subdivided into 5 layers, while the upper and the lower annulus into 4 and 2 vertical layers respectively.

These control volumes are connected with 136 atmospheric junctions, necessary for the simulation of the mass and heat exchanges among the various vessel zones. Moreover, in ASTEC, 41 drain junctions were also employed to simulate the condensate water drain, connecting the upper and lower annulus and the outer volumes of dome, inner cylinder and bottom area to their respective discharge volumes. On contrary, MELCOR has not a proper drain junction model, then the film tracking model was employed to simulate the condensate water route to the external volumes.

The vessel walls have been modeled with 136 heat structures, 76 simulating the h/c jackets (24 the lower, 30 the middle and 22 the upper h/c jacket). The carrier oil has been simulated as a “solid slab” instead of a “flowing fluid”, as requested in the benchmark specifications.

This quite detailed nodalisation has been developed to allow the investigation of the natural circulation phenomena among the main ThAI vessel zones.
In the following two cases for each code will be reported, differing for the external boundary conditions imposed in the input data. The cases for each code are slightly different due to the different conditions that can be imposed in the input decks. The four cases are here listed:

- the “ASTEC-K” is characterized by an outer wall temperature and an outer heat transfer coefficient calculated by the code;
- the “ASTEC-T” is characterized by an outer heat transfer coefficient forced at 5 W/m²K and by an outer wall temperature set to 20 °C;
- the “MELCOR-K” is characterized by an outer heat transfer coefficient forced to 5 W/m²K. In this case the outer wall temperature is calculated by the code;
- the “MELCOR-T” is characterized by and imposed outer wall temperature set to 20 °C. In this case the outer heat transfer coefficient is calculated by the code.

![Figure 2. Nodalisation scheme.](image)
6. Results

In the following the main thermal-hydraulics results of the ThAI Iod-12 test are reported. In particular, the analysis is mainly focused on the total pressure, the local atmosphere temperatures, and the local relative humidity, which are the most important parameters to achieve a good Iodine behaviour simulation [7].

6.1. Total pressure

![Figure 3. Total pressure in the dome area (7.7 m).](image)

The total pressure was measured at 7.7 m inside the dome area (figure 3). As shown, the total pressure trend is similar in all the four cases till the end of the mixed phase, while in the following phases a quite large difference is shown.

A slightly pressure peak underestimation during the mixing phase characterizes the four cases. This difference is around 0.2 – 0.3 bar for the ASTEC cases, while for the MELCOR cases this underestimation does not exceeds 0.15 bar. An insufficient heat exchange with the outer environment during the late phases of the tests affects the ASTEC-K and MELCOR-K cases, leading to a total pressure overestimation of about 0.3 – 0.4 bar. On contrary, the ASTEC-T and the MELCOR-T cases follow the experimental trend without major discrepancies.

As conclusion it can be stated that both the ASTEC-K and the MELCOR-K cases are unable to predict the experimental trend, while ASTEC-T and MELCOR-T are in good agreement with the experimental data.

6.2. Dome temperature

The atmospheric temperature has been measured at various heights during the Iod-12 test. In figure 4 the atmospheric temperature inside the vessel dome at 8.4 m is reported.

The four cases show a similar trend till the begin of the rest phase, while in the following the influence of the imposed boundary conditions starts to be relevant. The MELCOR-K cases present the maximum temperature difference (8 °C) among the calculated data and the experimental data during the first 12 h of the test. In the rest and the resuspension phases both the ASTEC-K and the MELCOR-K cases show a quite large overestimation of about 35.0 – 40.0 °C. On contrary, both the ASTEC-T
and the MELCOR-T cases follow without major discrepancies the experimental trend. However, during the final resuspension phase also these two cases present a slight overestimation of about 8.0 °C for the MELCOR-T case, and of 15.0 °C for the ASTEC-T case. This final discrepancy is probably due to the wrong temperature redistribution inside the vessel, being the total pressure correctly predicted during this phase (see above paragraph).

6.3. Inner cylinder temperature

In Figure 5 the atmospheric temperature inside the inner cylinder at 5.6 m is shown. The atmospheric temperature inside the inner cylinder zone is probably one the best indicator of the correct mass and energy redistribution among the inner and outer vessel zones.

As shown in the graph all the 4 cases are able to predict extremely well the temperature trend till the end of the mixed phase, while on the rest and the resuspension phases some discrepancies are reported. In detail, the MELCOR-T and the MELCOR-K cases suffer for an insufficient heat exchange toward the outer zones of the vessel, leading to a temperature overestimation during the rest phase which influences also the final resuspension phase. Moreover, the trend of the MELCOR-T case is continuously decreasing instead of being “flat”.

On contrary, the ASTEC-K and the ASTEC-T cases are closer to the experimental data for the entire transient. A slight overestimation is shown in ASTEC-K case starting from 14.0 h, leading to a total error of 10 °C at the end of the resuspension phase, while the ASTEC-T case does not suffers major discrepancies during the entire test. As conclusion it could be stated that the ASTEC-T is the only case in which the redistribution of mass and energy among the vessel zones is well predicted.

![Figure 4: Atmospheric temperature inside the dome area (8.4 m).](image-url)
6.4. Relative Humidity

The relative humidity has been measured at three eights during the test. In Figure 6 the relative humidity at 8.4 m inside the dome area is reported.
The differences among the cases here reported are quite large. The ASTEC cases are both characterized by a complete underestimation of the r.h., especially in the mixing, the mixed, and the rest phases. This underestimation is around 40% for the ASTEC-K cases, while for the ASTEC-T the magnitude of this underestimation changes during the various phases of the test, from around 40% in the mixing phase, to about 10% at the end of the rest phase. Moreover, in the ASTEC-T case the r.h. trend during the rest phase is different compared to the experimental one. Therefore, it should be stated that both the ASTEC cases are unable to correctly predict the r.h. values and trend during the Iod-12 test.

On contrary, the MELCOR cases are closer to the experimental data values and trend, but large discrepancies can be highlighted during specific phases. The mixing phase is well predicted by the MELCOR-T case, while the MELCOR-K case is characterized by a global overestimation leading to an almost saturated condition from ~6.0 h to ~7.0 h. During the mixed phase both cases shown the same behaviour, but in the rest phase the trends became different, in particular the MELCOR-K trend becomes similar to that of ASTEC-K case, and the MELCOR-T case becomes similar to that of the ASTEC-T case. However, in the MELCOR cases the global underestimation respect to the experimental data is lower, reaching and error not larger than 20%. Finally, the resuspension phase is characterized by larger underestimation in all the four cases, therefore, it could be stated that except for the MELCOR-T case all the other three cases are unable to correctly predict the r.h. trend in the Iod-12 test.

6.5. Helium concentration

The helium concentration has been measured at various heights during the Iod-12 test. In figure 7 the helium concentration at 8.7 m is shown. It should be highlighted as the experimental data provided are characterized by several uncertainties [4]. First, they refer to a steam-free atmosphere, therefore the concentrations shown after 5 h are slightly overestimated. Second, the initial peak is a local effect; hence its simulation is quite difficult. Therefore, the comparison between calculated and experimental data should be based on overall trends instead of a pure values comparison.
As shown, the four cases here reported show similar trends during the first 15.0 h, but in the latest hours of the test the ASTEC-T and the MELCOR-T cases report a continuous helium concentration increase, while the ASTEC-K and the MELCOR-K trends are similar to the experimental one.

7. Conclusions

As conclusion of this work it can be stated that the new versions of the ASTEC and MELCOR codes are able to predict the thermal-hydraulics transient of the ThAI Iod-12 test, but proper boundary conditions should be provided. In particular, it seems that the best choice is to let the code calculates the heat transfer coefficient instead of imposing an user-value. Moreover, it should be highlighted that heat transfer coefficient has a preeminent influence on the overall thermal-hydraulics results, as clearly shown in figures 3 and 4. Nevertheless, a good thermal-hydraulics simulation is needed for proper Iodine calculations, because the main phenomena involving Iodine are strongly influenced by the local thermal-hydraulics conditions. In particular the Iodine deposition and resuspension mechanisms are strongly influenced by the local r.h. values and by the local wall temperatures, therefore these two parameters should be as closer as possible to the experimental data.

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