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Main outcomes of OECD/NEA THAI-2 project and its use for code validation and containment safety assessment under accident conditions

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ABSTRACT

During a core-melt accident, apart from hydrogen, radioactive gases and aerosols are released into the containment, the behaviour of which is of significant importance for determining the radiological source term. The investigation on in-containment combustible gases and fission product behaviour was subject of the OECD/NEA THAI-2 project conducted during 2011 - 2014. The project focused on experiments on hydrogen behaviour i.e., deflagration in the presence of spray and mitigation by passive autocatalytic recombiners (PAR), on the interaction of molecular iodine with reactive and non-reactive aerosol particles to assess the effect on a potential source term, and on the quantification of the release of gaseous iodine from a flashing jet, representing a PWR steam generator tube rupture during reactor shutdown. The project was supported by 11 countries involving safety organizations, research laboratories and industries.

The experimental programme of the OECD/NEA THAI-2 project strongly contributed to the validation and further development of advanced lumped parameter and computational fluid dynamic codes used for reactor applications by e. g. providing experimental data for code benchmark exercises. The present paper summarizes main findings of the project together with highlighting their importance for mitigation of hydrogen risk and source term related issues. Furthermore, use of project results by the project partners for code validation and reactor analyses towards management and mitigation of a severe accident in light water reactors is discussed with selected examples.

KEYWORDS

Hydrogen risk, source term, mitigation systems, SGTR, THAI facility

1. INTRODUCTION

During a core-melt accident in a nuclear power plant (NPP), hydrogen and radioactive fission products are released into the containment, the latter as noble gases, gaseous iodine and aerosols. A series of complex phenomena involving hydrogen and fission products then occur, according to various accident scenarios and the prevailing boundary conditions. For accident management purpose, the engineered safety systems and passive mitigation systems, such as Spray and Passive Autocatalytic Recombiners (PARs) are designed

to prevent the accumulation of hydrogen and also to curtail any adverse consequences of hydrogen combustion on radioactive material release into the environment. Despite of significant progress achieved in understanding hydrogen and fission product phenomena, a number of safety relevant gaps in this understanding exist due to limitations in the experimental data bases. The need to investigate and understand the hydrogen behaviour in the containment compartments as well as the effectiveness of mitigation measures under postulated severe accident conditions has also been affirmed by the nuclear accident at the Fukushima-Daiichi plants. Similarly, the behaviour and the distribution of fission product iodine can be affected by a variety of chemical and physical phenomena taking place inside the containment. For this purpose, both large scale experiments reasonably representative of dominant accident sequences and accident simulation tools validated against experimental data are necessary for the analysis of the containment response during accidents and also for the effective planning of accident management measures.

In this context, the joint nuclear safety research project OECD/NEA THAI-2 was launched in 2011 for the duration of three years. The project consortium included technical safety organizations, research centers, regulatory bodies, industry, and universities from 11 countries, namely; Canada (AECL, now CNL), Czech Republic (UJV Rez), Finland (VTT, STUK), France (IRSN), Germany (BT, FZJ, AREVA, NIS, RUB, GRS, RWTH), Hungary (NUBIKI, PAKS), Japan (JAEA), Korea (KAERI), Netherlands (NRG, VROM), Sweden (SSM), UK (HSL, ONR).

The project aimed to investigate open questions related to the behaviour of hydrogen, iodine, and aerosols in the containment of water-cooled reactors during severe accidents. The project contributed to the validation and further development of advanced Lumped Parameter (LP) and Computational Fluid Dynamics (CFD) codes with 3D-capabilities used for reactor applications, e.g., by providing experimental data for code benchmark exercises.

2. WORK PORAGRAM

As part of the project work program, the following experiments were conducted:

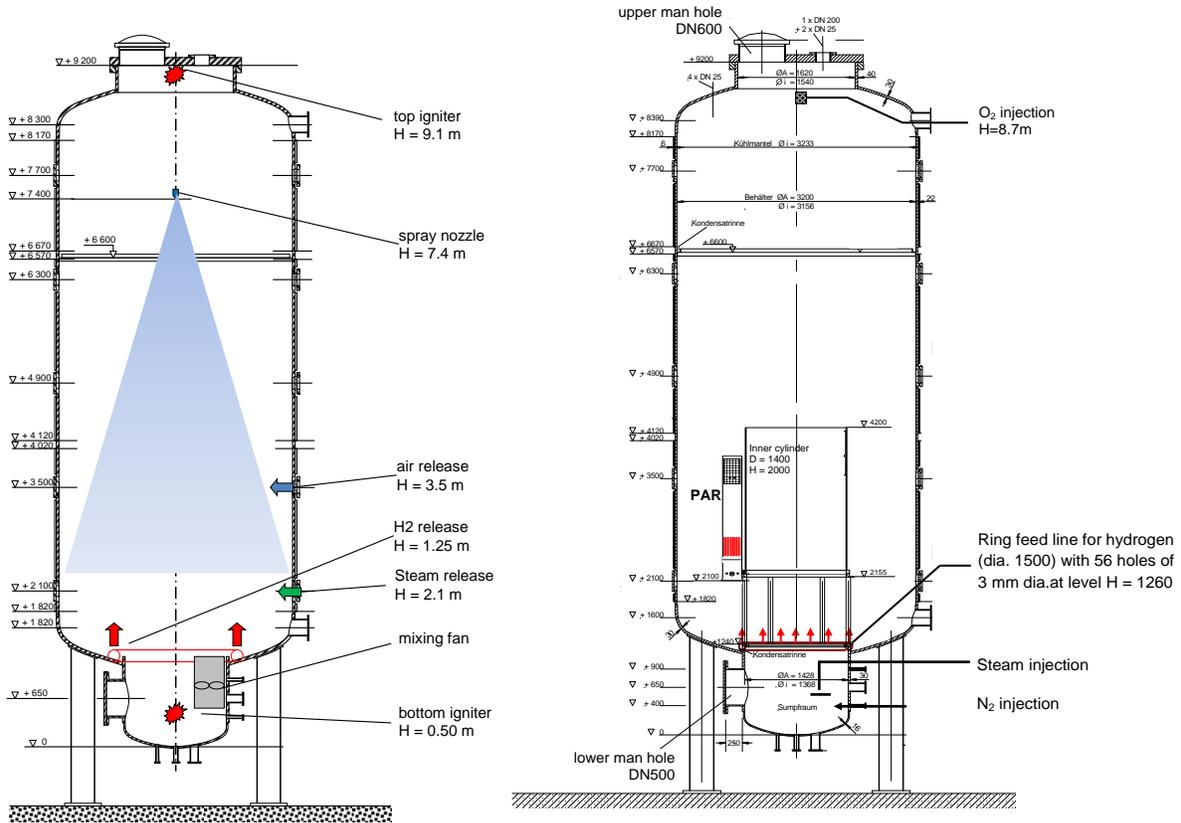
- Hydrogen deflagration during spray operation (HD),
- PAR performance at extremely low O₂ concentrations (HR),
- Interaction of molecular iodine with reactive and non-reactive aerosols (Iod),
- Release of gaseous iodine from a flashing jet, SGTR DBA scenario (Iod),
- Laboratory scale experiments on the interaction of iodine and aerosols.

In addition to the experimental work, an analytical working group (AWG) was established in the project framework. The AWG activities were aimed at the evaluation of the test results to provide support in further development and validation of predictive capabilities of advanced LP- and CFD-codes currently in use in the reactor safety field. Furthermore, AWG organised a code benchmark exercise based on hydrogen recombiner test HR-35 that involved both blind and open post-test calculations phases.

3. TEST FACILITY

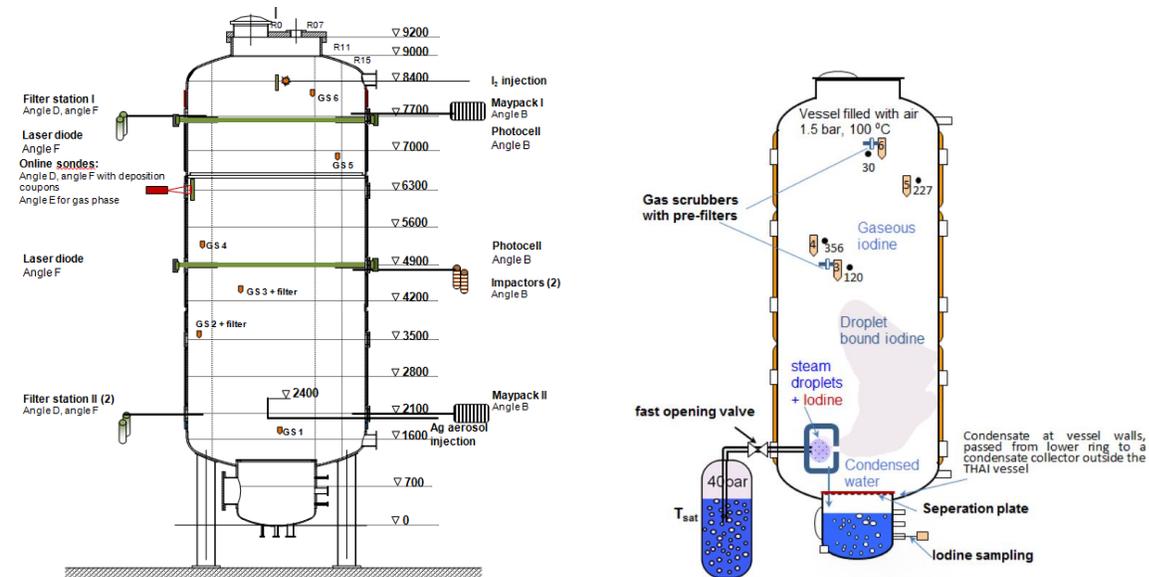
The experiments have been performed in the technical-scale THAI (Thermal-hydraulics, Hydrogen, Aerosols and Iodine) containment test facility (a 60 m³ stainless steel vessel 9.2 m high and 3.2 m in diameter with exchangeable internals) designed for multi-compartment investigations. The vessel is designed for a maximum overpressure of 1.4 MPa at 180 °C and can withstand moderate hydrogen deflagrations. The facility is operated by Becker Technologies GmbH at Eschborn, Germany in close co-operation with GRS (Cologne, Garching) and Framatome (Erlangen).

Fig. 1 shows various configurations of THAI test facility used for conducted the experiments mentioned above in section 2. Even though the facility is designed for containment specific investigations, integral tests requiring coupling with boundary conditions relevant to reactor cooling systems can also be conducted by installing auxiliary hardware (e.g. Iod-29 test, Fig. 1d).



(a) Hydrogen deflagration tests (HD)

(b) Hydrogen recombiner tests (HR)



(c) Iodine/Aerosol interaction tests (Iod-25&Iod-26)

(d) Iodine flashing test (Iod-29)

Figure 1: THAI test facility configurations in OECD/NEA THAI-2 project

The facility is equipped with the necessary supply systems for steam, compressed air, nitrogen, oxygen, light gases (helium and hydrogen), aerosols and gaseous iodine, the latter also radioactive traced with I-123 (half-life of about 13.5 hours). The vessel walls can be heated and/or cooled to establish the desired thermal hydraulic conditions including both well-mixed and stratified gas atmospheres.

To provide relevant database, an advanced instrumentation and data acquisition system is installed to monitor the relevant physical quantities with high spatial and time-related resolution. Selected measurement techniques installed for the experiments conducted in the frame of OECD/NEA THAI-2 project are mentioned below:

- Gas flow velocity by turbine flow meters in vessel gas atmosphere and at PAR inlet.
- A grid of “fast” sheathed thermocouples (outer diameter 0.5 mm), installed at 13 different elevations in the test vessel to monitor flame propagation (“flame front arrival”) and flame temperature during hydrogen combustion.
- The transient deflagration pressure is monitored by four “fast” pressure transducers (1 kHz) of the strain gauge type.
- Aerosol filter stations for aerosol concentration measurement.
- Laser light extinction for on-line aerosol concentration measurement.
- Cascade impactors for aerosol particle size distribution measurement.
- Gas scrubbers for gaseous iodine concentration measurement.
- Maypack filter stations for the discrimination of the iodine species in the vessel atmosphere.

4. MAIN OUTCOMES

4.1. Hydrogen deflagration during spray operation (HD)

The primary function of spray operation is to remove heat and condense steam in order to control pressure and temperature in LWR containments. Unfavourable effects of spray operation might be steam condensation which increases the volumetric concentration of the hydrogen with the threat of a more severe combustion in case of an ignition, and enhanced gas turbulence generated by the falling droplets which increases flame speed and combustion completeness. Quantitative data on the influence of spray droplets as well as spray induced flow conditions on hydrogen combustion in a large-scale test facility are required to verify and enhance current spray/combustion modelling capabilities.

In THAI HD test series, the sufficiently large volume of the test facility allowed to study the effect of spray induced flow (turbulence) on upwards and downward flame propagation behaviour. The specified tests conditions and varied parameters in the tests are shown in Table 1. In order to quantify the effect of spray on flame propagation behaviour, hydrogen deflagration tests conducted with similar initial thermal-hydraulic conditions but without spray (HD-7, HD-22 & HD-23) were used as reference tests from OECD/NEA THAI project [1].

All tests have been conducted with pre-mixed flammable mixture prior to activation of spray. The spray operation was initiated once the specified initial thermohydraulic conditions, i.e. temperature, pressure and gas composition were established in the test vessel. Tests were conducted with single full-cone spray nozzle installed at the elevation of 7.4 m and with spray angle of 30 °C (Fig. 1a). The spray water mass flow rate used for all tests was 1 kg/s. For studying the gas atmosphere mixing and cooling effects, two different nozzles with spray droplets Sauter mean diameters (SMD) of 670 µm and 970 µm were used. The spray operation was started 2 s before the onset of ignition to facilitate achieving stationary flow conditions for flame propagation. The only test with spray duration different than 2 s was HD-35 that was conducted with an extended duration of 60 s. For HD-35 test with hot spray water, despite of longer spray duration, no condensation occurred but a slight vaporization, since the vessel atmosphere was at superheated conditions.

Table 1: Specified tests conditions for HD-tests together with reference tests HD-7, HD-22 & HD-23

Test parameters	HD-30	HD-7	HD-31	HD-31-SE	HD-32	HD-33	HD-22	HD-34	HD-35	HD-23
Vessel pressure [bar]	1.5	1.5	1.5	1.5	1.5	1.5	1.5	1.5	1.5	1.5
Gas temperature [°C]	20	25	90	90	90	90	90	90	90	90
Hydrogen content [vol %]	10.0	10.0	10.0	-	10.0	10.0	10.0	10.0	12.0	12.0
Steam content [vol %]	-	-	25	25	25	25	25	25	25	25
Spray water Temperature [°C]	20	-	20	20	90	90	-	20	90	-
Spray droplet size, [µm], SMD	600	No Spray	600	600	600	600	No Spray	900	600	No Spray
Burn direction	Up	Up	Up	No burn	Up	Up	Up	Up	Down	Down

Fig. 2 shows pressure evolution over time for deflagration tests with and without spray operation. For a H₂ concentration up to 10 vol. %, all HD-tests with spray and upward combustion (Fig. 2, Left) exhibited clearly a suppressing effect with respect to peak pressures and peak temperatures. Only for the test with downward burn conducted with 12 vol. % hydrogen (Fig. 2, Right)), in which flame travel and spray induced flow had the same direction, combustion peak pressure was about 10 % higher than for the reference test without spray, but clearly below the respective adiabatic-isochoric-complete-combustion (AICC) pressure.

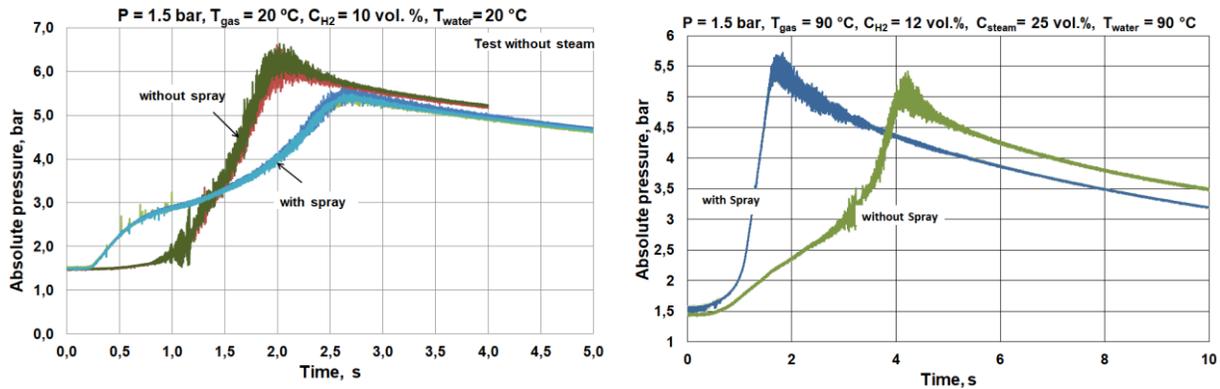


Figure 2: Pressure evolution in tests with and without spray: Upward burn (left), Downward burn (right)

From reactor application perspective, it can be expected that this effect weakens for gas mixture with 10 vol.% H₂ (mostly used upper requirement for hydrogen management in containments), which is less sensitive to flame acceleration. On the other hand, containment typical multi-compartment geometry may result into high local pressure loads at relatively low hydrogen concentration, as observed at H₂ concentration of 9 – 10 vol. % in a specific test configuration with two inter-connected compartments of BMC facility [2].

In general, THAI tests show that a higher degree of combustion completeness occurred in the test with spray. For the flame quenching process, the total available droplet surface is a decisive parameter. Spray nozzle with large droplet size indicated less cooling effect, enhanced gas mixing and consequently slightly increased pressure. The variation in spray water temperature indicated no observable effect on combustion suppression.

4.2. PAR performance at extremely low O₂ concentrations (HR)

In the course of a reactor accident, the oxygen content of the containment atmosphere can run low either locally or globally e.g., due to increasing steam content or by preceding H₂-O₂ reaction of operating PARs. As a consequence, PAR recombination performance can be degraded rendering relatively more hydrogen available in containment atmosphere in case of controlled or uncontrolled releases to the environment. Moreover, as discussed above, gas composition will differ significantly in between early and late phases of an accident. The ternary diagrams used in assessing the hydrogen risk based on the prevailing gas mixture are generally based on air/steam/hydrogen gas mixture system, which needs to be adapted if gas mixture system differs, e.g., for the late phase of MCCI due to reduced O₂ content in air.

In the above-mentioned context, the HR test series aimed to evaluate the influence of initial thermal-hydraulic conditions (gas temperature, pressure) and gas composition (H₂/O₂/steam concentration, O₂/N₂ ratio) on PAR performance, such as start-up, recombination rate, depletion efficiency and ignition behaviour. The specified initial test conditions for HR tests conducted by using two different commercially available PARs are shown in Table 2.

Table 2: Specified initial tests conditions for HR tests

Test ID	P [bar]	T [°C]	Steam content [vol %]	O ₂ content [vol %]	H ₂ content [vol %]	PAR type
HR-33	1.5	105	-	< 0.5	4	AREVA
HR-34	2.0	105	40	< 0.5	4	AREVA
HR-35	3.0	117	60	< 0.5	4	AREVA
HR-36	1.5	69	20	< 0.5	10	AREVA
HR-37	1.5	90	30	< 0.5	10	AREVA
HR-38	2.0	105	40	< 0.5	4	NIS
HR-39	3.0	117	60	< 0.5	4	NIS
HR-40	1.5	117	-	air	-	NIS
HR-41	2.0	105	40	air	-	NIS
HR-42	3.0	117	60	air	-	NIS

The test matrix consisted of three sets of tests, i.e. HR 33-35 and HR 38-39 investigating PAR start-up and performance behaviour under extremely low O₂ conditions; HR-36 & HR-37 investigating the effect of O₂/N₂ ratio on PAR ignition behaviour, and HR 40-42 investigating PAR performance behaviour under different thermal-hydraulic conditions. The test conditions in Table 2 refers to the start time of H₂ injection for tests HR 33-35 & HR 38-39, and to the start time of O₂ injection for tests HR-36 and HR-37. In case of experiments starting with nearly inert atmosphere (below 0.5 vol. %), the test vessel was purged by nitrogen. Thereafter, H₂ was injected until the target concentration of 4 vol. % was established, followed by a pulse release of O₂ to quantify the onset behaviour and later on by a continuous O₂ release until O₂ concentration at the PAR inlet reached about 2 vol. %. For tests HR 40-42, test procedure consisting of two tests phases as used for majority of the HR tests in OECD/NEA THAI project [1] is followed.

The PAR performance is assessed based on the following parameters derived from measurements:

- O₂ surplus ratio (Φ) defined as $\Phi = 2 * C_{O_2}/C_{H_2}$; $\Phi = 1$ means stoichiometric O₂-H₂ ratio at PAR inlet.
- H₂ recombination rate calculated by use of data measured at PAR: inlet temperature, inlet flow velocity, inlet/outlet gas concentrations, and the vessel pressure. Alternatively, recombination rate was determined based on the hydrogen mass balance over the entire vessel.
- H₂ depletion efficiency (in %) is calculated from the measured H₂ concentrations at the PAR inlet and outlet, i.e. $(C_{H_2in} - C_{H_2out}) / C_{H_2in} \cdot 100$.
- Dilution ratio defined as $\delta = O_2 \text{ conc.} / (N_2 + O_2) \text{ concentration}$ corresponding to $\delta = 0.21$ in air.

The effect of extremely low oxygen concentration on PAR start-up and performance behaviour is quantified by comparing the results with reference data under sufficient O_2 surplus conditions for the same recombiner type [1]. Under sufficient oxygen surplus conditions, when H_2 was released into an air or steam-air atmosphere, the recombination onset occurred at 0.2 – 4.4 vol.% H_2 depending on the initial temperature, pressure and steam concentration. In the present tests, the start-up behaviour of PARs was not affected by extremely low O_2 concentrations. The start-up was almost immediately when exposed to increasing oxygen concentration by injecting a pulse (< 0.5 vol.% concentration at PAR inlet) under nearly inert atmosphere containing hydrogen. However, lean oxygen concentration is shown to adversely affect PAR (designed) capacity of hydrogen recombination. A minimum oxygen surplus ratio Φ of 2.2 (AREVA), 2.3 (AECL) and 2.75 (NIS) was required for the PAR to operate at its design capacity [1]. At $\Phi = 1$, the PAR capacity fell below 50 % of the design capacity. Hydrogen recombination is mainly governed by available O_2 for $\Phi \leq 1$.

In an oxygen lean atmosphere ($\Phi < 2$), the depletion efficiency was less than 50 %, but increased linearly with an increase in the oxygen surplus ratio. Above an oxygen surplus ratio value of $\Phi = 2$, further increase of hydrogen depletion efficiency becomes very small and remains between 50 - 70 %. Fig. 3 (left) shows hydrogen depletion efficiency for OECD THAI-2 tests together with reference tests from OECD/THAI project [1], in which oxygen depletion occurs due to continued PAR operation. For oxygen surplus ratio value $\Phi > 2$, a hydrogen lean gas mixture prevails at the PAR inlet and the rate of recombination is mainly governed by the rate of hydrogen diffusion through the catalyst boundary layer.

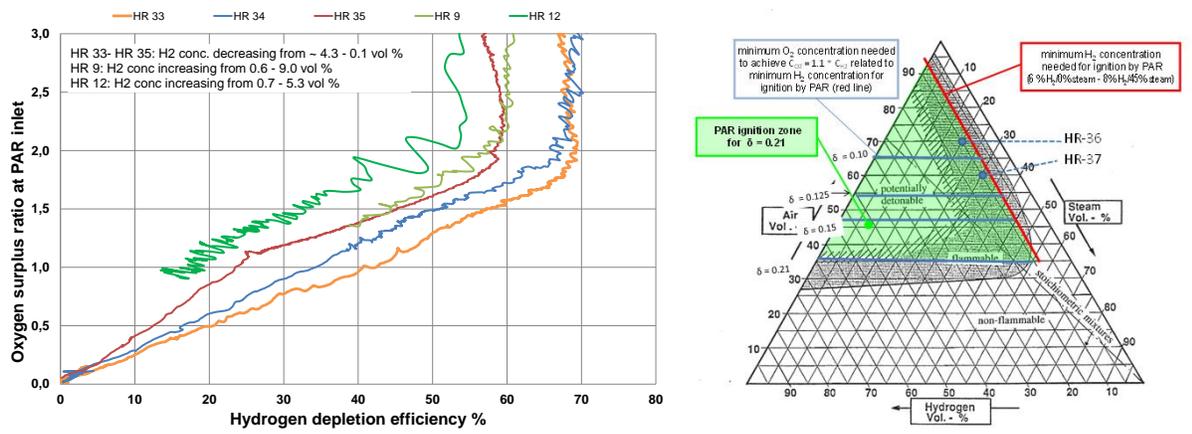


Figure 3: PAR performance: H_2 depletion efficiency as a function of O_2 surplus ratio (left), and flammability limit of the H_2 - O_2 - H_2O system for different dilution ratios (right)

Experiments conducted with sufficient O_2 surplus ratio have revealed that ignition occurred as soon as a critical level of hydrogen concentration at the PAR inlet ranging between 6.0 (for dry mixtures) and 9.0 vol.% (for mixture containing 45 vol. % steam) has been reached [1]. In oxygen lean mixtures, the concentration of oxygen is the limiting factor for the hydrogen recombination rate and results in lower catalyst temperatures if O_2 starvation conditions are reached. PAR induced ignition potential in O_2 lean mixtures is low, since the catalyst temperatures are directly correlated to PAR self-ignition. Tests HR-36 and HR-37 provided validation database for PAR ignition behaviour under gas composition containing different O_2/N_2 ratio than air, Fig. 3 (right). It was shown that in the oxygen starvation regime (oxygen surplus ratio below $\Phi = 1.5$ for dilution ratio below 0.21) and with the H_2 concentration sufficiently high (> 9 vol % at PAR inlet), ignition is very sensitive to the conditions and requires that the oxygen transient renders the gas mixture flammable at PAR inlet, above the catalyst within the PAR, and in the vessel. Other than that, catalyst surface temperature and gas temperature above the catalyst needs to be high enough to allow flame propagation in the H_2 , O_2 -depleted and steam enriched mixture above the catalyst.

4.3. Deposition of gaseous iodine onto reactive and non-reactive aerosols

The interaction between molecular iodine (I_2) and aerosols (non-reactive or reactive) is one of the issues lacking data for code validation purposes. It is one of the competing processes to the I_2 /paint interaction and hence of significant influence on iodine source term. Aerosol bound iodine might remain long term airborne compared to gaseous iodine.

It was the objective of the experiment Iod-25 to show whether at all or to which extent the inert SnO_2 aerosol is influencing the gaseous I_2 and how much I_2 will be trapped by the aerosol.

The test Iod-25 was run in 3 main phases, always at around 70 °C, air atmosphere, and at slightly increased pressure above atmospheric pressure. At the beginning of the first test phase (21 h), 1.0 g gaseous I_2 , labelled with I-123, was injected and its slow deposition onto the steel walls of the THAI vessel was monitored as a background process to the relevant interaction of I_2 with SnO_2 particles during the subsequent two aerosol test phases. The second test phase (5 h) was initiated by a short-term, maximum-power aerosol injection, followed by monitoring the evolution of aerosol and iodine in the vessel atmosphere. The third test phase (5 h) contained a long-term aerosol injection in order to maintain a nearly constant aerosol concentration at a medium concentration level. A very well controlled and very efficient SnO_2 aerosol injection was realized using a fluidized bed reactor. Gas scrubbers and Maypack filters were the main instrumentations to monitor the iodine in the vessel atmosphere. Scintillation detectors in front of deposition coupons were measuring the iodine deposition on steel and on SnO_2 -loaded steel. Aerosol concentrations were measured by filters and laser diode, aerosol sizes by impactors.

The maximum aerosol concentration after the first aerosol injection was 2 g/m³, the mean concentration during the second test phase was 1.15 g/m³. The mass median diameter (MMD) was 1.2 µm in both aerosol injection phases.

The results of the gas scrubber and Maypack measurements (Fig. 4, left) show a slow decline of atmospheric iodine concentrations. It is attributed to the reaction of I_2 with the steel of structural components. A stronger decrease was seen after the two aerosol injections. Speciation measurements with Maypacks (Fig. 4, right) revealed that the vast majority of iodine was found in the I_2 fraction and only a small part as aerosol-bound iodine. Although the aerosol-bound iodine fraction appeared to be low during Iod-25, the atmospheric iodine concentration determined from numerous samplings from the vessel atmosphere is clearly decreased due to the removal by the so-called "inert" SnO_2 aerosol. The iodine mass balance, based upon the sum of iodine washed from the vessel after the test and from iodine removed by the numerous samplings during the whole test, is closed (99 %).

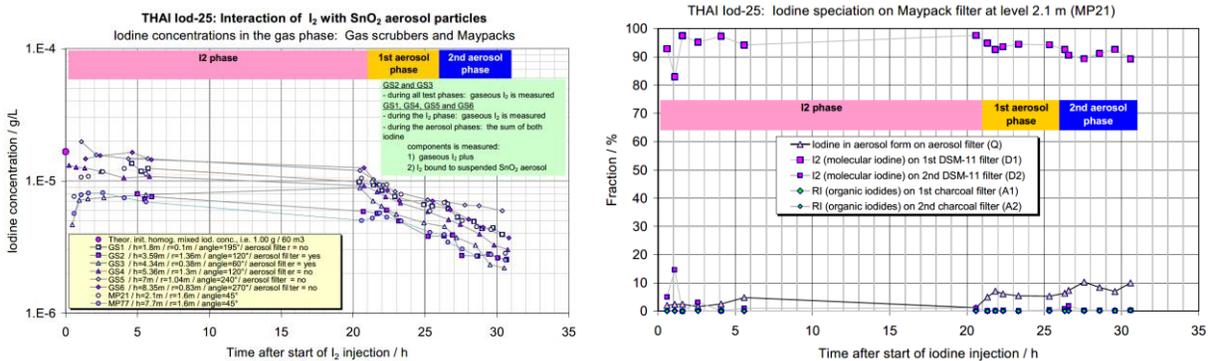


Figure 4: Iod-25 test: Measurement of gaseous iodine concentration (left), and measurement of iodine speciation based on Maypack measurements (right)

The Iod-26 test dealt with the interaction of molecular iodine with Ag (reactive aerosol). It has been conducted with silver (Ag) aerosol representing reactive aerosol material. Ag aerosol can be expected in the containment from molten Ag-In-Cd control rods.

The test Iod-26 was run similar to Iod-25, in 3 main phases, always at around 70°C, air atmosphere, and at initial vessel pressure of 1.5 bar. At the beginning of the first test phase (19.5 h), 1.0 g gaseous I₂ was injected and its slow deposition onto the steel walls of the THAI vessel was monitored as a background process to the relevant interaction of I₂ with Ag particles during the subsequent two aerosol test phases. The second test phase (2.5 h) was initiated by a short duration Ag aerosol injection, followed by monitoring the evolution of aerosol and iodine in the vessel atmosphere. The third test phase (5.6 h) contained a long-term aerosol injection in order to maintain a nearly constant aerosol concentration at a medium concentration level.

The maximum aerosol concentration after the first aerosol injection was 1.2 g/m³, the mean concentration during the second test phase was 0.50 g/m³. The mass median diameter (MMD) was 1.1 μm in both aerosol injection phases.

All measurements of atmospheric iodine species, total atmospheric iodine concentrations, and iodine loadings on stainless steel and silver surfaces provided a consistent view on the significant I₂/Ag aerosol interaction. In contrast to the previous SnO₂ test Iod-25, Maypack speciation measurement reveals that iodine is predominantly in an aerosol-bound form already immediately after the first aerosol injection in Iod-26, Fig. 5. The fraction of I₂ physisorbed on Ag aerosol particles is very low, unlike with the "inert" SnO₂ particles in test Iod-25, so I₂ resuspension from particles is largely suppressed in the Ag case. The gaseous iodine concentration is efficiently decreased due to the removal by the reactive Ag aerosol. Assuming that settling of iodine aerosol is the dominating process for the removal of iodine from the vessel atmosphere, a mean settling rate of 7.7E-4 m/s was determined for the total of both aerosol phases. This is 4 times faster as compared to test Iod-25 with the inert SnO₂ aerosol.

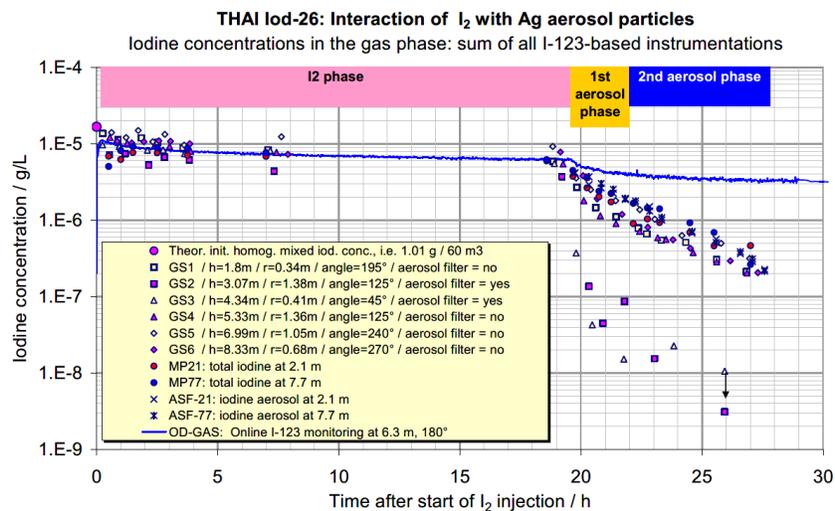


Figure 5: Iod-26 test: Evolution of gaseous iodine concentration before and after aerosol injection

Tests Iod-25 and Iod-26 can be considered to provide the bounding cases for the effect of I₂ removal from atmospheres by interaction with aerosol, the reactive Ag aerosol providing the maximum and the inert SnO₂ the minimum removal rates under the given boundary conditions of the tests. Real containment aerosol can be expected to show removal effects lying between these bounding cases, depending on its surface reactivity defined by the chemical phases available for reaction with gaseous I₂. With respect to application in severe accident containment models, the evaluation of the Iod-25 and Iod-26 data will require more detailed kinetic

models and a coupled iodine / aerosol interaction model would need to be included. Such a model is also required to assess the general significance of the I₂/aerosol interaction in severe accident source term calculations and thus to assess the need for further experimental studies, e.g., mixed/multi-component aerosols, effect of steam.

4.4. Release of gaseous I₂ from a flashing jet (Iod-29)

The iodine flashing test Iod-29 aimed at investigating a specific design basis accident (DBA) scenario in the event of a steam generator tube rupture (SGTR). The release of primary coolant from a SGTR leak occurs as a two-phase flashing jet, and this could represent an additional source for gaseous iodine in the containment. The THAI test Iod-29 was the first experimental approach to quantify the amount of gaseous iodine released during flashing.

The THAI vessel was initially filled with dry air at 1.50 bar and 100.3 °C, the sump was filled with 310 L decalcified water. A separate pressure vessel (PV), connected to the droplet separator inside the THAI vessel via a 9 mm release line, was filled with 750 L water, buffered to pH 7.1±0.1 (1E-2 mol/L KH₂PO₄, 6.7E-3 mol/L NaOH). A pre-fabricated I₂ nugget to be dissolved during heat-up was placed in a specific fixture and inserted into the cold water of the pressure vessel. Pressure vessel heating to 247.0 °C, 40.17 bar started right afterwards and lasted for 9.3 h. The iodine concentration in the PV water before flashing was 1.84E-2 g/L iodine. Flashing, initiated by opening the fast-opening valve, lasted 3.03 min and finally 2.85 bar, 122.9 °C in the THAI vessel and 38.64 bar, 245.6 °C in the pressure vessel were obtained. During flashing, 178 kg of water was drawn from the pressure vessel, of which ≈41 kg steam was generated and transferred to the THAI vessel. ≈137 kg water was directly transferred during to the THAI sump, the thermodynamic flashing evaporation rate is ≈23 %.

In the THAI vessel atmosphere, iodine sampling was permanently performed for 4 hours after start of flashing by 4 gas scrubbers, of which two (GS3, GS6) were equipped with pre-filters to retain water droplets and two (GS4, GS5) left without pre-filters. The gas scrubbers were operated with an absorber solution of 4 g/L NaOH and 7.85 g/L Na₂S₂O₃ · 5 H₂O.

Post-test iodine measurement of the samples by ICP-MS revealed that no gaseous iodine above the detection limit could be found in the THAI vessel atmosphere after flashing. (One datapoint at t=0.68 h was found to be inconsistent with the set of all other measurements and, since no plausible explanation other than a cross-contamination was found for it, considered as an outlier.)

This finding is supported by iodine speciation measurement by ion chromatography in the PV water, where only iodide was found, but no iodate concentrations above the detection limit of 5.4 % with respect to the sum of all iodine species (total iodine). A modelling study [3] confirmed the non-existence of a significant gaseous iodine fraction under the conditions of THAI test Iod-29 whereas at more representative conditions, a significant fraction of volatile inorganic iodine species would be expected. The need of further experimental research to validate and further improve the mechanistic iodine chemistry models was identified under conditions covering high temperature and low concentration with and without irradiation effect.

5. APPLICATION OF PROJECT RESULTS – MODELLING AND REACTOR CASE

The experimental database developed in the frame of the OECD/NEA THAI-2 project has been extensively used to validate and further improve safety analyses codes for containment analysis. The codes have been based on different modelling approaches, e.g. LP, CFD, Mechanistic. The analytical activities performed by the project partners provided comprehensive analyses of the experimental data by carrying out pre- and post-test calculations of the conducted tests. The validated codes together with improved models have been successfully applied for reactor analysis purposes. Table 3 summarizes a selection of THAI data application by the project partners for modelling improvement and reactor application purposes.

Table 3: Application of OECD/NEA THAI-2 project results by the project partners

Organization	Application of project results
GRS (Germany)	<ul style="list-style-type: none"> • Re-evaluation of PAR concept in German PWRs with revised PAR model AC²/COCOSYS. Efficiency of the installed PAR concept confirmed. • Validation of plate-type PAR model of GRS for NIS-PAR using THAI-2 HR data and identification of further modelling needs. • Application of HD tests data to check and align specific input variables of the COCOSYS combustion model. Validation of CFD modelling against HD data – identification of lack of models for flame extinction (Codes: AC²/COCOSYS and CFX) • Assessment and identification of need to improve modelling of the I₂/Ag-particle reaction in COCOSYS-AIM for dry and wet condition
UJV (Czech Republic)	<ul style="list-style-type: none"> • To support in assessment of a PARs based mitigation system installation in the Temelin Nuclear Power Plant containment (MELCOR code)
IRSN (France)	<ul style="list-style-type: none"> • Extension of PSA studies and accident modelling by including PAR-induced ignition behaviour results (SPARK and ASTEC codes) • Application of safety analyses codes based for calculation of hydrogen combustion in complex geometry (FLUENT and ASTEC codes) • Implementation of reaction mechanisms between gaseous I₂/non-reactive & I₂/reactive aerosols in safety analyses code ASTEC • Model development work based on identified lack of modelling in the existing iodine chemical models in the aqueous phase – high temperature chemistry (ASTEC)
JAEA (Japan) & NRA (Japan)	<ul style="list-style-type: none"> • Estimation of gaseous iodine adsorption velocity on aerosols derived based on tests data for application in BWR SA analysis (ART code) • Application of tests data for customization and validation of a non-nuclear H₂ safety analysis code for calculating flame propagation in LWR containments (FLACS code)
KAERI (Korea)	<ul style="list-style-type: none"> • Enhancement and validation of CFD codes capability to predict the effect of spray operation on hydrogen combustion (CFX code)
KINS (Korea)	<ul style="list-style-type: none"> • Implementation of an improved correlation for hydrogen recombination rate calculation of NIS-PARs to cover both early and late phase of an accident. Application of tests data to assess the predictive capabilities of codes for PAR performance under a broad range of accident conditions (e.g., O₂-lean, counter-current) (CFX and MELCOR codes)
VTT (Finland)	<ul style="list-style-type: none"> • Assessment and further improvement of hydrogen combustion modelling in CFD codes (FLUENT code)
CNL (Canada)	<ul style="list-style-type: none"> • Application of tests data in verification and validation of the general requirements for CANDU containment safety analysis, e.g., peak pressure, peak temperature, H₂ concentration in single-vessel and multi-compartment geometries (GOTHIC code) • Assessment of PAR modelling implemented in safety analysis code GOTHIC for late phase of an accident (O₂ lean conditions)
PSI (Switzerland)	<ul style="list-style-type: none"> • Application of tests data to assess predictive capabilities of CFD and lumped parameter simulation tools for PAR performance under a broad range of accident conditions (FLUENT and GOTHIC codes) • Assessment of CFD codes for simulation of hydrogen combustion in LWR containments
NUBIKI (Hungary)	<ul style="list-style-type: none"> • Application of tests data for modifications in the NIS recombiner model implemented in safety analysis code ASTEC

The application of hydrogen deflagration test data for validation of LP and CFD codes revealed difficulty in reproducing turbulence enhancing effect by spray to correctly simulate spray and combustion interaction. For correct modelling of spray effects, it was considered mandatory to implement phase interactions between gas and droplets in CFD simulations. Work on development and further improvement of models included modelling efforts on calculating spray induced entrainment, heat and mass transfer between droplets and gas demonstrated significant progress, see e.g. [4, 5]. Analytical activities also identified lack of modelling to predict the flame quenching, which could occur due to high turbulence or heat losses.

For modelling of flame quenching behaviour, further efforts towards providing additional database and modelling improvements are currently in progress, e.g. hydrogen deflagration tests planned in two-vessel configuration in the presently ongoing THEMIS project [6].

Analytical activities related to hydrogen recombination under oxygen lean conditions were mainly directed towards refinement of PAR modelling and the associated code validation activities. As the test series provided both data specific to PAR performance as well as data on interaction of an operating PAR with the surrounding containment gas atmosphere, the analytical activities also benefited from data suitable to validate PARs based mitigation systems performance in full containment analyses. The code benchmark based on test HR-35 [7] addressed a large variety of modelling approaches used in simulation codes employed for containment safety analyses and for assessing the hydrogen risk. Specific to PAR modelling, the employed modelling approaches included user-defined correlations, PAR vendor correlations, and detailed mechanistic modelling, among others. The benchmark results revealed that in order to accurately predict the PAR performance behaviour, like start-up and recombination rate, a proper modelling of the released energy from an operating PAR and the correct prediction of natural convection through the PAR is necessary to ensure precise PAR inlet conditions. Satisfactory results were obtained by mechanistic models on prediction of PAR behaviour under O₂ lean conditions. The PAR vendor correlations showed large deviations to the experimental results at very low O₂ concentration conditions. However, it should be noted that under very low O₂ concentration conditions, absolute catalytic recombination of hydrogen is quite limited and the modelling effort would be large. Several partners attempted to refine empirical correlations implemented in codes for O₂ lean conditions. It was shown that modification in correlations require accurate calibration of modelling constants to calculate the PAR recombination rate accurately. Apart from PAR performance behaviour, the extended database on PAR ignition limit including both early [1] and late phase conditions as investigated in THAI-2 project provided useful input for Level-2 Probabilistic Safety Assessment for hydrogen risk analyses [8]. The studies performed by the partners revealed the benefit of considering data on PARs as source of ignition, e.g. to assess the consequences of PAR induced ignition in containment safety analyses [8, 9]. Following successful validation, the safety analyses codes have also been used for designing hydrogen mitigation system, e.g. for the containment of a VVER-1000 unit (Czech Temelin NPP) [10].

Not all modelling needs could be answered based on THAI-2 HR data. The remaining PAR modelling needs were identified [11] particularly corresponding to the effect of extended range of accident conditions on PAR performance. The topics of high priority on PAR performance investigation included adverse flow effects and combined effect of O₂-starvation and carbon monoxide. In this regard, the OECD THAI & THAI-2 PAR results together with new data and modelling activities being carried out in different project frameworks (e.g. SAMHYCO-NET[12], OECD/NEA THEMIS[6], EC/AMHYCO¹ continue to provide the useful basis for validation and further improvement of PAR models. A code benchmark to assess the combined effect of carbon monoxide and carbon dioxide under O₂ lean conditions on the PAR performance is part of the ongoing OECD/NEA THEMIS project.

Concerning fission product transport, the tests on iodine depletion on chemically reactive and non-reactive aerosol particles (Iod-25 & Iod-26) provided extension to existing knowledge and contribute to assessing the safety relevance of this effect. Based on the experimental data, the identified reaction mechanisms have now been implemented in safety analyses codes e.g., THALES2/KICHE[13], ASTEC[14], and AC²/COCOSYS [15] to consider iodine adsorption mechanism on aerosols in addition to other sink for I₂. To assess the applicability of results for reactor analyses purpose, reactor calculations performed by the partners covered different accident scenarios, e.g., total loss of steam generator feed water in PWRs [14] and station black out scenario in BWRs [13]. The reactor analyses outcomes showed that in order to correctly account for experimental results in reactor analyses, it is necessary to consider the results as bounding cases as reactor typical multi-component aerosols, possibly mixed with structure material may

¹ <https://amhyco.eu/>

render challenging conditions for interaction with gaseous iodine. Furthermore, overall gaseous iodine sink may also depend on characteristics of molecular iodine such as the gas/liquid mass transfer and the adsorption onto aerosol and structure surface. Nevertheless, experimental and the related analytical activities clearly revealed that after I_2 is adsorbed onto the aerosol surfaces, the behaviour of I_2 follows the aerosol dynamics. This change in the iodine behaviour might result in a significant influence on the iodine source term and needs to be considered in source term calculations.

The iodine flashing test Iod-29 demonstrated the complexity and sensitivity of this process involving high temperature iodine chemistry. There were successful efforts by project partners, e.g., to develop a simple thermal-hydraulic model to calculate the flashing rate and the droplet size distribution providing satisfactory results but calculation of iodine chemistry part was quite uncertain [3]. Codes had difficulty in matching the experimental observation that the injected molecular iodine reacted quickly with the steel wall of the primary vessel during heat-up and thus, had produced the non-volatile iodide form. More experimental and analytical work will be needed in future to accurately account for on aqueous phase iodine chemistry effect in source term calculations.

Some of the remaining open questions after OECD/NEA THAI-2 project have been addressed in the follow-up OECD/NEA THAI-3 and the presently ongoing OECD/NEA TEHMIS project. In THAI-3 project issues related to investigations on PAR performance under counter-current flow conditions and to hydrogen deflagration experiments in a two-compartment system under natural convection flow regimes. Additionally, in the light of the Fukushima Daiichi accident, experimental investigations are foreseen to study the release of fission products (aerosols and gaseous iodine) from a water pool at elevated temperature (as a consequence of continuous water heating or venting induced boiling (depressurization)). Another experiment was related to the “delayed source term” and shall investigate the resuspension of aerosols as well as iodine deposits from steel/painted surfaces due to hydrogen combustion. The ongoing THEMIS project aims to investigate hydrogen combustion/mitigation (PARs) and source term related issues and provides experimental database under representative “late phase conditions”, such as CO , O_2 lean atmosphere, elevated pressure/temperature, steam.

6. CONCLUSIONS AND PERSPECTIVES

The overall objective of the OECD/NEA THAI-2 project was to investigate open questions concerning the effects of operating safety and mitigation systems spray and PARs on hydrogen risk mitigation and the behaviour of iodine and aerosols in the containment of water-cooled reactors during severe accidents.

The project served to provide experimental data on the deflagrative combustion of hydrogen during operation of a spray system in the containment, and on its removal by means of passive autocatalytic recombiners in oxygen lean conditions, as well as on their ignition behaviour. Regarding the interaction of gaseous iodine with inert and reactive aerosol, the experiments focused on the quantitative determination of the iodine-aerosol interaction and the deposition of aerosol-bound iodine. In addition, the release of gaseous iodine from a depressurized water-steam mixture (simulation of SGTR during a reactor shutdown) was investigated.

The project contributes to the further development and validation of computational models used in reactor safety research by, among other things, providing experimental data for HR-35 test based benchmark exercises. Furthermore, the project serves to maintain competence in the field of reactor safety in the OECD/NEA member countries and promotes international cooperation between these countries.

As a perspective, future THAI programme will continue to provide database useful for severe accident management and code validation purpose. Moreover, opening to other research areas, such as investigations on passive safety systems in advanced reactor technologies (including SMRs) is also possible to be addressed in the THAI facility with eventual development of new features.

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