The International Test Programme in the THAI Facility and its Use for Code Validation

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Abstract:
The focus of the paper is on selected results of the extended experimental containment research program at the THAI facility in Eschborn, Germany, and its use to validate lumped parameter (LP) and field (CFD) codes with the aim to improve or develop physical models for different phenomena relevant to accident and severe accident conditions in NPP. Experiments in the areas of nuclear reactor containment thermal hydraulics, hydrogen, aerosol and iodine (fission products) behavior have been conducted. The recently launched national THAI IV test program and further planned international activities are outlined at the end of the paper.

The THAI program is performed by Becker Technologies GmbH, Eschborn, in close cooperation with AREVA NP GmbH, Erlangen and the technical departments of Gesellschaft für Anlagen und Reaktorsicherheit (GRS) mbH, Cologne. Experiments in the THAI facility began in 2000 under the sponsorship of the German Federal Ministry of Economics and Technology, following the traditions of German containment research in the large-scale facilities BMC (Battelle Model Containment) and HDR (Heissdampfreaktor). The German national part of THAI Phase III (2006 - 2009) has been completed, the international part performed in the frame of an OECD-NEA THAI Project (2007 - 2009) with sponsors from Canada (COG-AECL), Czech Republic (NRI), Finland (STUK), France (IRSN), Germany (GRS), Hungary (VEIKI), Korea (KAERI), the Netherlands (VROM) and Switzerland (PSI) will be finished by the end of 2009. So far, two OECD International Standard Problem (ISP) exercises using experimental results form the THAI facility have been conducted respectively are ongoing.

For the THAI experiments, coupling of thermal hydraulics, fission product transport and chemistry is a main focus, especially for iodine with its high radiological importance. In support of CFD code development, the experimental program is based on a strategy of successive enhancement of complexity, beginning with simple forced flow field investigations, then stepwise adding other physical interactions like buoyancy, heat exchange, and steam condensation. THAI results have been used in code development or validation of numerous containment codes - LP codes: COCOSYS, ASTEC, MELCOR, CONTAIN, TONUS-LP, FUMO, KUPOL-LP as well as CFD codes: GOTHIC, GASFLOW, TONUS, KUPOL, DEFINE, CFX, FLUENT, STAR-CD. The German containment code system COCOSYS is currently the main code used to test new or improved models mainly related to the iodine topic. A transfer of such new models into the integral code ASTEC under common development at IRSN and GRS is also planned.

1 OBJECTIVES OF THAI RESEARCH

1.1 THAI project history

Experiments in the THAI vessel began in 2000 under the sponsorship of the German Federal Ministry of Economics and Technology, following the traditions of German containment research in the large-scale facilities BMC (Battelle Model Containment) and HDR. Since 2007, the national THAI research program is rounded off by the OECD THAI project with 8 international partner countries from Canada (COG-AECL), Czech Republic (NRI), Finland
THAI results have been used in code development or validation of numerous containment codes (LP codes COCOSYS, ASTEC, MELCOR, CONTAIN, TONUS-LP, FUMO, KUPO-LP; CFD codes GOTHIC, GASFLOW, TONUS, KUPO, DEFINE, CFX, FLUENT, STAR-CD). Code comparison benchmarks with THAI test data have been conducted for different phenomena as gas stratification or hydrogen combustion, both, on the German national level (test TH7) and on the international level (OECD ISP-47 & ISP-49, OECD THAI HM-2 benchmark) as well. Further THAI results are utilized for iodine model validation in the frame of the European SARNET project.

1.2 THAI project objectives

An overview of THAI investigation topics linked to the four main topics - thermal hydraulics, hydrogen, Aerosol and iodine - is shown in Figure 1 and explained below in detail.

Figure 1: THAI investigation topics

1.2.1 THAI - Thermal-hydraulics

The basis for the containment behaviour is the thermal hydraulics which determines the thermodynamic states and the transport processes. In advanced models, the containment is represented by means of multiple control volumes in order to simulate inhomogeneous atmospheric distributions; for homogeneous conditions, a single-volume model would be sufficient. The thermal hydraulic THAI experiments focus on inhomogeneous atmospheric conditions, which most often show up as long-term stable atmospheric stratification. Formation and removal of a stratification are dependent upon distributed sources of heat and mass, like e.g. buoyant steam or hydrogen plumes from a primary system leak. The
atmospheric stratification has an impact upon transport and distribution of hydrogen and fission products in the atmosphere. In a couple of counterpart tests, the equivalence of helium as experimental replacement gas for hydrogen has been demonstrated under stratified conditions. Selected results of code validation related to thermal hydraulic aspects are presented in chapter 3.1.

1.2.2 THAI - Hydrogen

Safety related aspects of hydrogen are e.g. the structural loads from hydrogen combustion and the performance of passive autocatalytic recombiners (PAR). Multiple combustion events may occur during continuous hydrogen release, and it is necessary to estimate the combustion completeness under such conditions in order to assess the potential of turbulent flame acceleration. Data from THAI experiments help developing model correlations in this field, and they are used for validation of mechanistic flame propagation codes. The focus of the hydrogen deflagration experiments is on flame propagation in mixtures with low hydrogen concentrations, at various atmospheric conditions for vertical burn directions.

Recombiner performance was investigated under adverse conditions, where a lack of data exists. There is also a test series to investigate the potential of PARs as ignition source, in order to support the assessment of PAR installations as being safety-directed. Selected results of code validation related to hydrogen aspects are presented in chapter 3.2.

1.2.3 THAI - Aerosol

A more detailed knowledge of fission product transport processes in the containment is needed for the source term assessment in case of core meltdown accidents. Lab scale experiments contribute information on individual interactions, but cannot simulate the interactions of physical transport and chemical processes in a realistic accident scenario. A substantial step towards more realistic conditions is provided by the THAI fission product experiments. The size of the facility allows studying the combined effects of physical advection-dispersion in the atmosphere, mass exchanges at walls and water surfaces, and chemical reactions with structural surfaces or materials dissolved in water. Experience from code validation often shows that experiments with coupled effects behave different from hand calculations or code predictions which are based on theoretical synthesis of interacting phenomena. While THAI does not reach the complexity of chemical conditions as e.g. in the PHEBUS-FP tests, it can provide much more detailed information on spatial interactions, which is needed to validate multi-node simulation models. Selected results of code validation related to aerosol aspects are presented in chapter 3.3.

1.2.4 THAI - Iodine

Fission product research at the THAI facility has a major focus on iodine. The transport behavior of iodine components in the containment is strongly influenced by the interactions of gaseous iodine with walls and water bodies. From the first series of iodine experiments, a thorough understanding of the interactions between gaseous I₂ and the stainless steel walls of the THAI vessel has been developed. Based on this knowledge, subsequent experiments were conducted with painted walls by using reactor-typical coatings. Current and future experiments address interactions of iodine with ozone and aerosols, thermal formation of volatile I₂ from CsI when passing a hot PAR, wash-down of fission products from structural surfaces by water condensate flow, and pool scrubbing topics. Selected results of code validation related to iodine aspects are presented in chapter 3.4.
2 THAI FACILITY OVERVIEW

The THAI facility (Figure 2) for nuclear reactor containment research is intended to conduct experiments in an intermediate scale between separate-effects (laboratory tests) and integral effects (large scale tests). It is a multi-purpose facility which allows studying transport phenomena driven by natural convection, coupled to physical and chemical interactions of fission products, under thorough control by a high spatial density of measurement transducers in a single- or multi- compartment geometry. In particular, it is possible to conduct experiments with aerosols, iodine, and tests with passive autocatalytic recombiners under natural flow conditions. The data are used for validation and development of LP and CFD containment codes.

Figure 2: THAI test vessel and instrumentation

The vessel dimensions are: height of 9.2 m, diameter of 3.2 m, free volume of 60 m³; pressurization up to 1.4 MPa at 180 °C. The vessel walls are made of stainless steel with an outer thermal insulation and cooling/heating jackets for thermal control of wall temperatures.
Internal structures like an inner cylinder or horizontal separation plates are configured according to experimental needs.

As compared to other containment test vessels of similar size like MISTRA or PANDA, THAI has the unique possibility to work with combustible gas mixtures to study hydrogen recombination or slow deflagration; furthermore, it is suitable for investigating iodine transport and chemistry using a radioactive iodine tracer isotope. The spatial resolution of the measurements is higher than e.g. in the PHEBUS-FP containment simulator vessel, giving more detailed data for code validation related to spatial transport processes.

3 SELECTED RESULTS FROM THE THAI PROGRAM USED FOR CODE VALIDATION

3.1 Experiments on THERMAL HYDRAULIC behaviour

3.1.1 Atmospheric stratification with helium (ISP-47)

In the OECD International Standard Problem ISP-47 [Allelein 2007], THAI experiment TH13 was used to benchmark the capabilities of LP and CFD containment codes for simulating atmospheric gas distributions. A stratified atmosphere was generated by subsequent injections of helium and steam in the upper part of the test vessel. Then, the stratification was partly removed by buoyant steam flow from the lower injection port. The residual stratification persisted after terminating the injection. Test configuration and vertical helium concentration profiles are shown in Figure 3.

Figure 3: Results of atmospheric stratification test TH13 and blind predictions

Comparison of experimental data and results from blind code predictions showed that all CFD codes (CFX, DEFINE, GASFLOW, GOTHIC, designated as field codes in Figure 3) and
most of the LP codes (MELCOR, CONTAIN, TONUS-LP, FUMO, KUPOLO, ASTEC (IRSN model), COCOSYS (RUB model)) failed to predict the persisting stratification. This was somehow unexpected for the CFD codes because they solve a more complete set of conservation equations and make use of a finer mesh. The more successful LP simulations were based on an engineering approximation of the buoyant plume, implemented in the relatively coarse nodalization mesh. The latter approach had been developed earlier [Kanzleiter 1996, Fischer 2003] but received relatively little public attention.

The findings from ISP-47 gave rise to a more extensive investigation of the phenomena that govern the dissolution of an atmospheric stable gas stratification. Measurements with higher spatial resolution shall help identifying shortcomings and improving models in the CFD approach.

3.1.2 Atmospheric stratification with hydrogen (HM-2 benchmark)

As compared to ISP-47 [Allelein 2007], a partly simplified test procedure was applied in the HM test series, and the instrumentation was enhanced in order to obtain more detailed information about the light-gas-cloud erosion. Experiment HM-2 was selected as subject of a code benchmark. Participants from 11 Organisations participated using the LP codes ASTEC, COCOSYS and MELCOR and the CFD codes FLUENT, GOTHIC and GASFLOW [Schwarz 2008]. The experiment HM-2 in the THAI containment test facility was run in order to investigate the erosion of a stable atmospheric stratification layer by a buoyant plume from below, which has a lower density than the stratification layer. The stratification was established by injecting hydrogen in the upper part of the test vessel. Results from this phase were published, and the stratification was simulated reasonably well. The data from the second phase, during which the atmospheric stratification is dissolved, were concealed until the simulation results were submitted. The buoyant plume was generated by steam injection in the lower part of the vessel. The steam release from the lower injection port continues until the stratification was removed completely (different to ISP-47). Figure 4 (left part) shows the experimental set-up.

![Figure 4: Experiments on flow distribution and dissolution of stable stratification](image)

Summarizing the HM-2 benchmark - as compared to ISP-47 - a progress is seen in the calculated results. Blind CFD and LP model simulations of this second test showed better
comparison with the experimental results. Such progress must be considered in view of the simplified test arrangement for HM-2 as compared to ISP-47. All contributions simulated well the development of the light gas stratification during the open phase 1 of the experiment, and all need a certain time span to dissolve the stratification during the blindly calculated phase 2. However in phase 2 of the experiment large differences show up. Several LP and CFD contributions have delivered reasonable to good predictions of phase 2, whereas the quality is individually different for the sub-phases 2a and 2b. It is possible to predict the erosion of a light gas layer by a buoyant plume; however there are larger uncertainties in the predicted time needed. Figure 5 shows the decrease of the calculated and measured hydrogen concentration at the top of the vessel during phase 2 of the experiment.

![Figure 5: Hydrogen concentration in dome (HM-2), elevation 8.7 m, phase 2; comparison of code predictions [Schwarz 2009]](image)

Like previous ones, this benchmark shows a significant user influence for LP as well as for CFD contributions. Several simulation features being the reason for deviations to the experimental results have been identified, offering the potential for improvement:

- In order to simulate the development and the dilution of an atmospheric stratification LP nodalisations should contain (1) sufficient detail in vertical direction and (2) nodes and flow paths modelling upward directed plumes.
- For CFD simulations the choice of adequate wall functions is needed. Some results have improved when a finer grid was chosen. On the other hand it was found that a too small aspect ratio (vertical to horizontal grid size) could lead to less favourite results. The time steps need to be small enough in order to conserve mass and energy.

3.1.3 Atmospheric stratification (further HM tests)

Experiment HM-1 was a counterpart test to HM-2 where helium was used instead of hydrogen. The comparison of the Helium - Hydrogen counterpart tests show that best correspondence of test conditions is achieved if the light gas release rates are configured to yield identical volumetric fractions. The longer stagnation phase and the lower erosion
velocity of HM-2 compared to HM-1 can be explained by the higher density difference of HM-2. Differences in the molecular weights, thermal capacities and conductivities as well as molecular diffusivities of the two gas species are less important if the volumetric light gas fractions are below 40% in most parts of the atmosphere. No new or additional phenomena have been observed in HM-1. Therefore Helium can be used as a substitute for hydrogen.

The middle picture in Figure 4 shows the configuration of a stationary blower test with a recirculating flow loop in the THAI vessel, the data of which have been used to validate the momentum transport solutions of several CFD models. Deviations between calculated and measured results mainly exist in the flow field downstream of the sharp-edged orifices between the condensate trays which require further analysis.

The right picture in Figure 4 shows the arrangement for a test where the stratification was dissolved by means of a momentum jet instead of a buoyant plume. This test allows validating the models for turbulent interactions at the stratification interface. The observed large CFD-code underpredictions of momentum-driven turbulence form a remarkable contrast to the large overpredictions of buoyancy-driven turbulence. These results are representative for several variants of the k-ε turbulence model and indicate some substantial shortcomings which should be removed by suitable extensions of the turbulence closure relations; this work is currently in progress.

3.1.4 **Blind prediction of thermal convection (TH21)**

Another series of experiments at the THAI facility, where thermal convection acts as driving mechanism to dissolve an atmospheric stratification, is indicated in Figure 6.

![Figure 6: Experiments on thermal convection and dissolution of stable stratification](image)

The left scheme in Figure 6 is the basic test where the flow patterns in the atmosphere and the heat transport processes are investigated. The cylindrical part of the vessel wall is heated in the two lower sections and cooled in the upper section. The differential wall heating leads to unstable stratification conditions in the vessel atmosphere which drives a convective flow loop. This test poses a challenge to CFD models by coupling momentum and heat transport, with buoyancy forces being distributed all over the vessel space.
In the middle picture in Figure 6, a light gas cloud is superimposed in the upper vessel plenum and will be subjected to dissolution by the convective flow circulation in the lower part. Finally, the right picture in Figure 6 indicates that the cloud in the upper vessel dome is generated by buoyant steam instead of helium; in this case, suitable models for steam condensation need to be activated in the CFD simulation models, which is a major task for CFD codes from non-nuclear industrial origin. The last two cases will be investigated in the recently launched THAI IV program.

The experiment TH21 was conducted in 2008. The results have not yet been published as blind prediction have been performed by different participants using LP (COCOSYS, ASTEC) and CFD (CFX) codes.

First results of the CFX-11 blind prediction performed by J. Stewering, GRS, are discussed below. Two grids (quarter of the ThAI facility with symmetry boundary conditions) with 24192 respectively 74173 elements have been used (Figure 7). Figure 8 shows as an example the results of a simulation at 11 hrs of the test process (phase 2 of the experiment). A stable temperature and pressure distribution was reached by the simulation, while the velocities show big fluctuations. Only a small influence of the element number on pressure, temperature and velocities was observed in this case.

![Figure 7: CFX-11 grid of THAI-21 (heater section in red, cooler section in blue) [Schramm 2009]](image)
3.2 Experiments on HYDROGEN behaviour

3.2.1 Slow hydrogen combustion (ISP-49)

The general objective of the hydrogen deflagration experiments at the THAI facility is to investigate hydrogen deflagrations at low concentrations with vertical flame propagation in a sufficiently large geometry under conditions typically for severe accidents. This includes:
- combustion in upward and downward direction,
- variation of hydrogen and steam concentration and initial temperature,
- combustion of mixtures with and without steam and hydrogen concentration gradients, i.e. the coupling of hydrogen distribution and combustion,
- detailed recording of flame propagation, pressure transients, temperature transients and combustion completeness.

The experiments will contribute to an improved understanding of hydrogen combustion phenomena and to the further development and validation of containment system codes.
The particular objective of the test HD-2R from the THAI facility and the ENACCEF tests used for the OECD International Standard Problem ISP-49 (open phase) is to provide experimental $\text{H}_2$-deflagration data from tests with typical accident conditions (intermediate steam content, elevated initial temperature), both for upward and downward burn direction.

Figure 9 shows the results of two THAI tests - one with upward and one with downward burn direction. At the same initial conditions the downward burn flamefront velocity is remarkably slower compared to the upward combustion. Furthermore, it can be observed that the burn direction is reversed in the lower part.

20 participants from 7 countries using the LP codes ASTEC and MELCOR and the CFD codes CFX and GASFLOW started to analyse the results of the tests provided for the open phase of the ISP-49. Results for discussion are not yet available. Blind post-test calculations of experiments (different than those of Fig. 9), also part of ISP-49, are underway.

3.2.2 Passive autocatalytic recombiner (PAR) tests

PARs are used in many pressurized water reactor containments for hydrogen mitigation. The THAI vessel is a suitable facility for investigations using a commercial PAR unit of technical size because its large vessel volume allows to establish natural convection flow during PAR operation. In addition the test conditions allow to simulate typically severe accident conditions with respect to pressure, temperature and gas composition.
Recent THAI experiments focus on three points of interest:

- **Onset of recombiner activity under adverse conditions**, i.e. at enhanced atmospheric humidity and in the presence of aerosols and poisons.
- **PAR efficiency under oxygen starvation conditions.** Most PAR recombination rate tests have been done under lean hydrogen conditions with sufficient oxygen available. Prior to the THAI tests, limited investigations were done under oxygen starvation conditions which result in a reduction of recombiner efficiency already at a slightly over-stoichiometric oxygen-hydrogen ratio.
- **PAR ignition potential.** Ignition by a PAR has occurred in several experiments at higher hydrogen concentrations. Since PARs are used to recombine hydrogen without flame ignition, such events appear to be undesired. Systematic data on the conditions for PAR ignition were not available in public literature, but are now after the THAI experiments have been completed. In the experiments also the location of ignition is identified and the intensity of the PAR-induced deflagration is determined.

The arrangement of the THAI facility for the PAR tests is shown in Figure 10.

![Figure 10: PAR test configuration and procedure for ignition experiment](image)

Results from previous PAR performance pre-tests are shown in Figure 11 for a commercial unit exposed to an air-hydrogen atmosphere. Recombiners start their operation under enhanced concentration, as indicated in the figure. Under reactor accident conditions, the conditions for PAR operation startup and recombination performance are less favorable than in a dry air-H₂ atmosphere. The results of the THAI PAR test series will be used to improve the validation of the recombiner models currently applied in the LP codes COCOSYS and ASTEC and in the CFD code CFX.

Commercial PARs of ARVEA (former Siemens) have been tested at several other facilities before as well as PARs from AECL and NIS. ARVEA provides the customers with a set of equations which allows the calculation of the H₂ and CO recombination rate dependent on the PAR type and the gas composition and pressure. These equations have been implemented into the LP codes COCOSYS and ASTEC already some time ago. The same equations have been added now to the CFD code CFX-11 by GRS. For a post-test calculation of experiment HR-2, the model and the grid set-up is shown in Figure 12.
Figure 11: H₂ recombination rates; results of THAI-PAR-1 performance tests at different pressure levels

Figure 12: PAR model developed for CFX-11 (left) and set-up of THAI facility by CFX-11 for HR-2 calculation (right) [Schramm 2009]

The PAR model in CFX uses outlet (green area at PAR bottom in Figure 12 left) and inlet (red area at PAR bottom in Figure 12 left) boundary conditions at the PAR itself. No detailed reactions are modelled inside the PAR. Only the heat losses to the PAR walls are simulated.
The AREVA equations are applied to calculate the recombination rate based on the conditions at the PAR inlet.

The grid used consists of about 100000 cells. The hydrogen injection is simulated by a ring with 56 holes at a lower position of the vessel. The inner cylinder which holds the PAR is modelled as well but not visible in Figure 12.

The first results achieved by the analysis are promising. Figure 13 shows the hydrogen concentration at PAR inlet (left) and PAR outlet (right) [Schramm 2009]. Differences are caused by the ARVEA equations on one side and by the accuracy of the flow and gas distribution calculation of CFX on the other side. Furthermore, the start of the recombination was defined to be at 2 Vol.% of H₂ as proposed by AREVA, while in the experiment the PAR reaction already started at about 1 Vol.% This value varies from test to test. This work is still ongoing.

![Figure 13: Hydrogen concentration at PAR inlet (left) and PAR outlet (right) [Schramm 2009]](image)

### 3.3 Experiments on AEROSOL behaviour

The behaviour of airborne fission product loaded particles in the containment needs to be understood to assess their contribution to the source term. One of the objectives of the THAI test program is to investigate the aerosol behaviour in the containment under realistic thermal hydraulic conditions. There are very different aerosol related processes, which in the short-, mid- or long term might contribute to the aerosol source term.

Some examples are given below describing different aerosol processes like wet and dry resuspension, gas to particle conversion or the interaction of aerosols and components – e.g. I₂ and recombiners and consequences so far investigated in the THAI facility.

Different aerosol generation techniques have been established to produce prototypical aerosols like evaporating CsI and other materials by means of an inductive furnace and subsequent recondensation by quenching; or brushing machines by brushing aerosols from solid e.g. SnO₂ pellets; or in case of soluble materials like CsI, LiNO₃ etc., by spraying solutions and drying the solution droplets to obtain residual dry particles.
A broad spectrum of aerosol measuring techniques for characterizing particles in the range of 0.1 to 10 micron like classical impactors, low pressure impactors and optical measuring systems have been applied as well as electrostatic classifiers and condensation nucleus counters for particles in the submicron range, as required for gas to particle conversion processes forming ultrafine particles e.g. the IOx formation due to the ozone – iodine reaction.

3.3.1 Wet resuspension

The release of radionuclides from liquid surfaces into the adjacent gas atmosphere can be important for aerosol source term considerations especially in the late phase of a severe accident. Droplet resuspension from water surfaces with solved or suspended fission products can contribute significantly to the aerosol source term as well. This may occur during pool scrubbing, in case of a water covered core melt or sump boiling due to permanent decay heat supply or due to a pressure decrease in case of containment venting.

The major contribution of droplets respectively their residuals which remain airborne due to their small size are from the so called film drops, discharged from the lamella of a bubble during the disruption process, while the bubble is resting at the fluid surface. Larger so called jet drops reach only a limited height before falling back. Film drops in a superheated atmosphere will dry out forming residual fine particles containing fission products at high concentrations.

Figure 14 shows the results of the THAI entrainment measurements in the experiments TH14 – TH17 compared to older data available from REST and KWU experiments. The entrainment is defined as the ratio of the mass flow of droplets released into the atmosphere above the pool versus the steam mass flow rate.

**Figure 14:** Entrainment as function of the gas velocity; experimental results
The THAI experiments for wet resuspension are of integral character. In comparison to other resuspension experiments like REST the pool surface is large. The size distribution of the ascending bubbles in the water has been successfully measured by means of pin probes. The released airborne particles have been measured in the dome of the THAI vessel by means of a differential mobility particle sizer and an ultrafine condensation particle counter.

In order to model the release of resuspended drops from bubbling pools, an empirical correlation has been developed [Dapper 2008] and implemented in the containment code system COCOSYS. The correlation was validated against the experimental results for wet resuspension as measured in the “boiling sump” experiments in the THAI facility, showing good qualitative and quantitative agreement with the experimental data.

3.3.2 Dry resuspension

Dry resuspension can increase the aerosol concentration in the containment atmosphere. Already deposited aerosol material can be re-released into the containment atmosphere by atmospheric flows induced by hydrogen deflagrations or by other phenomena like steam explosions. The objective of the THAI dry resuspension experiments was to provide a basis to assess the possible influence of this dry resuspension effect on the radioactive source term.

During the resuspension experiments Aer-1, Aer-3, and Aer-4 [Kanzleiter 2006], a vertical deflagration tube (8 m height) was installed in the THAI vessel. In a first step, CsI aerosol was injected into the dry vessel atmosphere, settling during a period of typically 24 hrs onto the inner, preferably horizontal surfaces. In a second phase, a H₂ deflagration was initiated in the deflagration tube by igniting a H₂-air mixture. The expanding combustion gases were released through a 2 × 50 cm² nozzle running over the horizontal aerosol loaded surface causing resuspension of CsI particles. Velocities in the range of 17 m/s up to 67 m/s across the deposition plate were achieved by deflagrations with different flame velocities.

The CsI aerosol was characterized by means of low pressure impactors, filter measurements, sedimentation coupons and others during the CsI injection preloading of the inner surfaces and during the resuspension event. The surface loading was measured before each deflagration. The resuspended aerosol material showed a bimodal size distribution.

The dry resuspension experiments Aer-1, Aer-3, and Aer-4 in THAI provided the data to validate a new resuspension model [Nowack 2007], developed to describe the conditions found under strong and very transient air flows as expected after hydrogen deflagrations. This model has been implemented in the GRS containment code system COCOSYS [Allelein 2007]. Along with the modified Fromentin model [Fromentin 1989] for resuspension under highly transient air currents, source term studies have been performed with COCOSYS. A generic COCOSYS dataset of a KONVOI-type reactor was used to calculate an accident scenario with a possible hydrogen deflagration. The calculations show that in case of a very strong deflagration which induces high flow velocities in all containment zones, the released aerosol mass can be increased up to a factor of 10, which demonstrates the relevance of the dry resuspension mechanism.

3.3.3 Interaction between CsI aerosol and passive autocatalytic recombiner (PAR)

The catalytic oxidation of hydrogen in PARs results in temperature levels at the catalytic surfaces which can reach 900 °C or more and leads to elevated gas temperatures up to several hundred °C in the gas flow passing these surfaces. Suspended CsI particles transported with the convective gas flow through PARs under such conditions can be converted into volatile iodine creating an additional source term of volatile iodine.
Considering even low conversion rates might lead to a significant influence on the concentration of gaseous iodine in the early phase of an accident when high CsI / I$_2$ ratios can be expected.

Aer-2 and Aer-5 are two technical scale experiments performed in the frame of a former German national THAI Program to study the PAR influence on the formation of volatile iodine deploying an original SIEMENS type PAR under realistic thermal hydraulic conditions [Poss 2008]. CsI aerosol has been generated by evaporating CsI in an inductive furnace and monitored by low pressure impactors and filters. The hydrogen concentrations in the test atmosphere reached up to 10.5 Vol%. A proved molecular iodine sampling and detection method has been applied to determine gasborne iodine concentrations. In these experiments a CsI to molecular iodine conversion rate of 3 % has been determined as being an upper limit.

In the French RECI experiments, conversion of metal iodides (CsI, CdI) to gaseous iodine up to 60% was observed [Deschamps 2003]. However, this experiment was done on a laboratory scale by means of an electrical furnace with e. g. H$_2$ and steam not present in the gas.. The thermochemical properties may be not closely representative for real PAR operation.

Based on the above findings, it became evident that a possible additional source of gaseous iodine by PAR operation requires to be investigated under realistic severe accident conditions. In the frame of the OECD THAI project, tests with a commercial PAR unit under more realistic severe accident conditions in terms of gas composition (steam, air, hydrogen) and thermal hydraulic conditions have been conducted. Cesium iodide (CsI) aerosol particles have been used producing high aerosol mass concentrations of several g/m$^3$. These tests are completed and currently under evaluation. Findings will be published in the near future.

3.3.4  PAR poisoning

The recombiner units are designed to operate under conditions corresponding to severe accident with respect to pressure, temperature, humidity and radiation. However, during a core damage accident, fission products entering into the containment building may have adverse effects on the performance of a PAR unit. Observations made during various experiments emphasize the need to carry out additional experiments for a clear decision on the possibility of PAR poisoning by fission products under severe accident conditions. In the frame of the OECD THAI project it was decided to perform a PAR poisoning test that should be considered challenging but conceivable in terms of severe accident conditions in a nuclear power plant. This test has been performed and is currently under evaluation.

3.4  Experiments on IODINE behaviour

3.4.1  Iodine deposition on steel surfaces

The THAI iodine tests performed so far provide a basis to understand the source term relevant I$_2$ behavior. Deposition of volatile I$_2$ on decontamination paint represents an important sink in a containment. There are components with stainless steel surfaces in reactor containments too, e. g. in special designs of thermal insulation, but painted surfaces are more important. Numerous laboratory-scale experiments were performed on that topic in the past [Sims 1997]. However, the role of thermal-hydraulics and the iodine transport from gas to wall is not representative in such small-scale tests and remained an open question. As a coupled effects test facility and with its technical-scale dimensions, THAI is suited to investigate such problems. The interaction of gaseous iodine with stainless steel surfaces in
the THAI vessel was investigated first, because a good knowledge of this interaction is needed for interpreting the subsequent experiments on I₂-paint interaction.

Main parameters influencing the I₂ deposition and desorption at stainless steel walls are temperature and relative humidity. These dependencies have been investigated in THAI. Based upon a series of tests a consistent model of I₂/stainless steel interaction was recently derived [Langrock 2008] and implemented into COCOSYS/AIM. The I₂/steel model consists of a sequence of two processes: An initial, fast and reversible physisorption process, followed by a chemical reaction at the steel surface, where physisorbed I₂ is converted into non-volatile ironiodide FeI₂, (“chemisorbed iodine”); the rate of this reaction step increases with relative humidity.

In these tests gaseous I₂ was injected into the gaseous phase of a single-compartment THAI vessel at constant and homogeneous temperatures, and the I₂ decrease due to wet deposition on dry stainless steel surfaces was measured at temperatures of 60 - 110 °C and relative humidities from 0 - 80 %. The red curve in Figure 15 shows the resulting global model result for I₂/steel interaction in THAI. In this test, I₂ interaction with steel was measured as function of relative humidity over a broad range of relative humidity from dry air up to superheated steam/air mixture.

![Figure 15: Comparison of COCOSYS I₂/steel model with data from THAI Iod-18](image)

The model will be further validated by I₂/steel adsorption/desorption tests with radiation as part of the current OECD-BIP project. A comprehensive I₂/steel model is also required for the interpretation of other large-scale measurements, e.g. Phebus-FP or RTF. It might also be used to quantify effects on the retention of iodine by reflective metal isolation surfaces.

3.4.2 Iodine deposition and desorption at painted surfaces

Secondly, as mentioned in the previous chapter, the deposition and desorption of I₂ at painted surfaces was investigated. Epoxy paint representative for painted walls of German containments, artificially aged to about 15 years, was used and exposed to temperatures
from 80 - 140 °C and relative humidities between 20 - 75 %. Although the steel surface area of the test vessel was ten times larger than the painted surface area of the test specimen, about 90 % of the I₂ was deposited on the painted surface.

Again an new model was developed and tested for COCOSYS/AIM. The I₂ deposition at the paint surface is described using an empirical two-step model analogous to the I₂/steel interaction [Langrock 2008]: an initial, fast and reversible physisorption process, followed by a chemical reaction at the paint surface, where physisorbed I₂ is converted into non-volatile chemisorbed iodine.

Figure 16 shows the comparison of the COCOSYS/AIM prediction with experimental data of THAI test Iod-15 performed at 100 °C and 45 % relative humidity. The agreement between the analyses and the experiment is very good.

Figure 16: Comparison of COCOSYS I₂/paint model with data from THAI Iod-15 considering simultaneous I₂/steel interaction at vessel walls

I₂ interaction tests with steel and painted surfaces under steam-condensing conditions have been performed recently. Model analyses with the I₂/paint system are ongoing; the wet I₂/steel model has been included in COCOSYS/AIM as well.

3.4.3 Iodine mass transfer between containment atmosphere and sump

In the long term of a severe accident, the release of volatile iodine by mass transfer from the sump into the containment atmosphere represents a major source of air-borne iodine inventory and may contribute significantly to the source term. Volatile iodine species such as molecular iodine (I₂) or organic iodides (RI) are transported from atmosphere to sump by mass transfer through the interfacial surface area gas/liquid. The process is reversible, unless the iodine is converted into non-volatile forms by chemical reaction in either of the two phases.
THAI test Iod-9 was performed with the objective to provide data on the I\textsubscript{2} deposition onto dry and wet stainless steel surface, and on the mass transfer of gaseous I\textsubscript{2} between a deep and a shallow sump. Gaseous iodine was injected at the start of the test into a superheated steam/air atmosphere at 90 °C with dry walls. Repartitioning of the iodine was observed in the gaseous phase, at the wall and in the sumps. In a washing phase steam was injected at two different rates. The wet I\textsubscript{2} deposition and the simultaneous transport with the drained off wall water film have been measured.

The test was recently analyzed within the THAI group of the European SARNET project, and valuable results were obtained by GRS (COCOSYS/AIM), IRSN (ASTEC/IODE) and AECL (LIRIC) on all aspects of the test [Dickinson 2008]. The decrease in the gaseous I\textsubscript{2} takes place at a nearly constant rate due to deposition at steel surfaces and conversion into FeI\textsubscript{2} (Figure 17). The three iodine codes reproduce the gaseous I\textsubscript{2} fairly well during the dry wall phase. In the washing phase, gaseous iodine measurements are scattering.

![Figure 17: Gaseous I\textsubscript{2} concentrations in THAI test Iod-9 and code calculations](image)

Iodine mass transfer into the sump and its behavior in the sump was another major objective of Iod-9 test. In the stagnant phase during the first 4 hrs, the sump developed a temperature stratification and shows an inhomogeneous iodine distribution (Figure 18), with the highest concentration near the water surface and the lowest at the bottom. The iodine distribution changed with time. The contribution of diffusion to the iodine transport within the stagnant sump is weak.

To model the gas-sump mass transfer, all three codes use the two-film model, requiring the input of the gas- and water- side mass transfer coefficients (MTC). These coefficients for containment sumps are currently roughly estimated and user dependent. The water side MTC, mostly dominating the overall mass transfer rate, depends strongly on the flow conditions in the sump. Correlations are required for coupling the iodine mass transfer coefficient with thermal-hydraulics.
3.4.4 Iodine/Ozone reaction

The radiation field in the containment atmosphere in case of a severe accident produces air radiolysis products. Ozone is one of these molecules which in turn oxidize gaseous I$_2$ into iodine oxides or iodine-nitrogen-oxide compounds of various stoichiometries [Vikis 1985]. Laboratory-scale experiments with radiation were performed [Funke 1999, Langrock 2005] and mechanistic and empirical models were developed [Dickinson 2003] to calculate the chemical reaction rate of iodine oxide formation. An important aspect of this radiolytic oxidation of gaseous I$_2$ is the formation of solid particles (gas-to-particle conversion) which has been studied in THAI.

In these tests ozone was used as a simulant for the oxidizing air radiolysis products. Two tests have been performed at 100 °C in a superheated steam/air atmosphere at a relative humidity of 50 - 60 %. After I$_2$ injection, ozone was added to study the impact on iodine evolution in the vessel atmosphere. In another test, the vessel was filled with ozone first before injecting gaseous I$_2$. The deposition behavior of the instantaneously formed iodine oxides (IO$_X$) was measured. Figure 19 shows the impact of ozone injection upon the total iodine concentration, gaseous I$_2$ plus particulate IO$_X$.

The first of two ozone injections at 3 hrs was weak and showed no significant effect on the total iodine in the vessel atmosphere. However, the second large ozone injection at about 5.5 hrs nearly stopped further iodine deposition on the walls by forming ultrafine (0.1 µm and smaller) IO$_X$ particles remaining airborne. The deposition of the fine IO$_X$ aerosol is significantly slower than the chemical deposition of the gaseous I$_2$.

In another test (Iod-14) with a 100-fold excess of ozone over I$_2$ confirmed the Iod-13 test results with the fast conversion from the gaseous I$_2$ state into the particulate IO$_X$ state.

These results had some influence on the revision of the evaluation method for iodine speciation filters ("Maypacks") under radiation conditions such as Phebus-FP tests or EPICUR tests [Girault 2008].
Three THAI tests (Iod-10, Iod-11 and Iod-12) have been performed to study the iodine behaviour in multi-compartment configuration [Weber 2006]. The vessel was sub-divided into five compartments using steel plates with defined openings. The main processes studied were: iodine transport with gas and water flows, $I_2$ adsorption/desorption onto/from steel with and without steam condensation, and $I_2$ mass transfer between atmosphere and sump. The complexity of the tests was gradually increased, starting with the dry air test Iod-10, a superheated steam/air atmosphere in test Iod-11 and steam condensation at walls in test Iod-12. In all tests, $I_2$ and helium has been initially injected into the upper compartment to support a stratified vessel atmosphere. Typical temperatures have been approx. 100 °C in the upper compartments, whereas all lower compartments have been kept at lower temperatures close to ambient temperature at the bottom. The transition phase was initiated by heating the lower parts of the vessel walls and by injecting helium near the bottom to achieve mixing. After reaching well-mixed atmosphere identified by homogeneous He mixing, this "well-mixed phase" was kept constant.

$I_2$ showed a clear multi-compartment-behavior. The evolution of the gaseous $I_2$ concentration in all three multi-compartment iodine tests looks similar. The Iod-11 results are taken as an example (Figure 20). During the stratified test phase, $I_2$ is kept completely within the upper compartment. $I_2$ homogenization within this compartment took about 2 hrs. The slow decrease of gaseous $I_2$ is due to deposition on the steel surfaces (about 58 m²) of this upper compartment. During the mixing phase, gaseous $I_2$ is slowly transported into the lower compartments. However, unlike He, $I_2$ is not well mixed at the end of the mixing phase. Retardation of $I_2$ mixing is due to the retention at steel surfaces on its way from the upper compartment downwards to the bottom. There is still non-homogeneous $I_2$ repartitioning even at the end of the "well-mixed phase", 24 hrs after $I_2$ injection.
Figure 20: Iodine in the vessel atmosphere during THAI iod-11

COCOSYS/AIM F2 correctly describes all essential aspects of the I₂ distribution in the five compartments (Figure 21). The overestimation of the I₂ concentration by about a factor of 5 at t = 10 h is ascribed to the fact that the I₂/steel model did not yet reflect adequately the chemisorption, i.e. the formation of non-volatile FeI₂ especially at high relative humidity. ASTEC/IODE calculations show similar results as COCOSYS/AIM, but larger differences to measured data due to a less detailed I₂/steel deposition model. The I₂/steel model was only recently updated, based upon the THAI database and is included in the next version COCOSYS/AIM 3.

Figure 21: Gaseous I₂ concentrations in test iod-11 calculated with COCOSYS/AIM
The THAI iodine multi-compartment tests clearly demonstrate the multi-compartment effect of non-homogeneous mixing, based upon interim storage of gaseous I\textsubscript{2} on surfaces. This effect needs to be considered in iodine source term assessments of LWR containments, otherwise these are not always conservative. The effect could be even more significant in LWR containments based upon the large surface areas covered by decontamination paint being very reactive towards I\textsubscript{2}. Inhomogeneous iodine repartitioning in the containment has implications on local dose rate and decay heat distribution, the latter in turn influencing thermal hydraulics, hydrogen distribution and aerosol behavior. THAI test Iod-11 was successfully reproduced 3 years later to demonstrate that the iodine results are reproducible under identical thermal hydraulic conditions.

4 SUMMARY

The possibilities of the THAI facility to investigate coupled effects phenomena have been demonstrated by means of different experimental setups, related to the fields of containment thermal hydraulics, hydrogen, aerosols and iodine, and their use for code validation and model development. THAI is best suited for experiments which cannot be conducted in small-scale laboratory vessels. THAI tests are characterized by situations where spatial inhomogeneous distributions and related transport processes are involved, like heat and mass transfer boundary layers between atmosphere and structural or water pool surfaces, natural convection, and aerosol sedimentation. In contrast to this, e.g. experiments on chemical kinetics of iodine components are more efficiently done on a laboratory scale. The transfer of experimental results to reactor conditions is mainly a problem of spatial scaling, while chemical reactions are independent of the spatial scale. The larger scale of the THAI vessel makes it possible to investigate accident phenomena in an atmosphere under natural convection which could not be established in a small lab apparatus. The intensity of natural convection at the geometric scale of a nuclear reactor containment is considerably larger than in THAI, but such scale-up is accomplished by means of code simulation. In this sense, THAI takes a specific position in the model development/validation chain, different from lab-scale tests, and experiments in this facility should be designed according to the scaling considerations indicated above.

Experiments with well-mixed atmospheric conditions like e.g. in the Phebus-FP containment simulator are suitable to validate single-node containment models. Multi-node containment models typically for codes like COCOSYS, ASTEC, MELCOR etc. are designed for simulating also the spatial variability associated with inhomogeneous distributions of heat and mass species in the atmosphere. Large geometries like real containment buildings provide more favorable conditions for the development of inhomogeneous distributions, as compared to small test vessels. In an inhomogeneous atmosphere, characteristic time constants of advective transport interfere with time constants of fission product deposition and chemical reactions. As a consequence, transient concentrations of airborne radionuclides can widely differ between a mixed and a stratified atmosphere. Containment model validation for the mixed case is not sufficient for scaling to reactor cases. THAI experiments are aimed at providing data for inhomogeneous atmospheric conditions.

The sequence of experiments in support of CFD code development and validation represents a stepwise increase of complexity from strongly simplified towards more reactor-like conditions. The overall goal of this work is to establish a CFD simulation method for nuclear reactor containment simulation that shall be able to calculate atmospheric thermal hydraulics more accurately than present LP codes. Simultaneously, the data can be utilized for further improvement of the engineering approach for buoyant flow in the framework of LP modeling. It is expected that this approach is applicable to any existing LP code including the integral codes ASTEC and MELCOR and will lead to results similar to what has been demonstrated.
successfully with COCOSYS. Nevertheless, the ISP-47 and the follow-up HM benchmark demonstrated the significance of the influence of the experience of the code user on the results. The results of such international cooperations will significantly contribute to enhance the users knowledge.

Future THAI experiments in the frame of the German national THAI IV programme, funded by the German Ministry of Economics and Technology, comprise BWR related experiments dealing among others with thermal stratification in the wetwell, condensation of superheated steam and other hydrodynamic problems. In the field of fission product behaviour, experiments on wet resuspension from a boiling sump at higher gas velocities will be performed as extension of earlier experiments in THAI II at lower velocities. Aerosol and iodine transport by wall condensate films is another currently highlighted topic. Further important issues of the experimental matrix are the influence of turbulence on the deposition of I$_2$, the iodine mass transfer sump/atmosphere and the iodine behaviour under the presence of various aerosol species in a multi-compartment system. Specific emphasis is given to experiments which serve for the validation of CFD codes.

A planned THAI OECD follow up project concentrates on graphite dust transport in a generic HTGR multicompartiment geometry after depressurization of the RPV. Fission products sorbed on graphite dust particles released into the confinement in the event of helium leakage are source term relevant. A further issue of the envisaged programme is the investigation of the potential release of volatile iodine from a flashing jet assuming an SGTR event during the reactor shutdown procedure, where substantially enhanced concentrations of iodine in the primary circuit coolant can result from iodine spiking effect. The interaction of I$_2$ and aerosols is a competing process to the I$_2$/paint interaction and hence as well of significant influence on the iodine source term. Experiments are foreseen to determine parameters on deposition velocities and re-suspension rates to/from aerosols. As a consistent extension of the presently almost completed OECD THAI project it is foreseen to perform tests to investigate the influence of temperature, pressure and steam on the onset of H$_2$ recombination in case of very low oxygen concentrations. The effect of containment spray operation on vertical hydrogen burns is also foreseen to be investigated with a small series of test runs arranged in a comparable way as the deflagration tests in the first OECD THAI program.
References


