Executive Summary

During a severe accident leading to core melt-down in a LWR plant, radioactive fission and activation products will be released into the containment atmosphere as gas, vapour or, to a great extent, adsorbed on aerosols, while the containment building serves as the final barrier to the environment. Due to the fact that time dependence and distribution of fission products and aerosols are of great importance for mitigating the consequences of a severe accident, e.g. to protect the integrity of the containment by venting, a detailed knowledge of fission products and aerosols behaviour and a relevant analytical prediction capability are required. Experimental results and code predictions can be used to quantify safety margins presently existing in the safety relevant systems of operating reactors, and to explore possibilities for Severe Accident Management (SAM) measures. For demonstrating the capability of current computer codes to model and to calculate the aerosol distribution and settlement in containment with sufficient accuracy, the OECD-CSNI decided to propose an additional containment aerosol behaviour standard problem.

Following an offer made by the Federal Republic of Germany, the OECD-CSNI agreed on its 1998 December meeting to make use of experiments taken from the KAEVER test series performed at Battelle GmbH, Eschborn, Germany for International Standard Problem No. 44. The ISP44 comprises four open and one blind KAEVER aerosol depletion tests with three differently soluble aerosol materials and uniform thermal hydraulic conditions with slight volume condensation. Concerning the blind case, besides initial and boundary conditions, the relevant experimental results had been locked and not delivered to the participants in the ISP prior to performing the calculation.

The preparatory meeting was organized by the Gesellschaft für Anlagen- und Reaktorsicherheit (GRS) mbH Köln, Germany in January 2000. 10 organizations from Europe, Korea and Japan
submitted their results for comparison and evaluation by using the codes ASTEC, COCOSYS, CONTAIN, MELCOR and ARTMOD2/REMOVAL.

ISP44 followed a series of former ISP in this area. The most related ones are ISP37 (VANAM M3 Aerosol Behaviour in the Battelle Model Containment), AHMED Code Comparison Exercise and different CEC benchmark problems.

The general objectives of the ISP44 were to analyze the aerosol behaviour, e.g. volume condensation and settlement of aerosols in a containment atmosphere with well defined thermal hydraulic boundary conditions.

In more detail the objectives of ISP44 were the comparison and investigation of the following physical variables and phenomena:

- State-of-the-art status review on computer codes for containment analysis, e.g. aerosol behaviour and partly, thermal hydraulics
- Phenomena and physical variables to be investigated:
  - Pressure in the test vessel
  - Atmospheric temperature in the test vessel and the vessel sump area
  - Wall temperatures inner and outer test vessel (insulated) and inner and outer doorway (not insulated)
  - Relative humidity
  - Volume condensation rate and water droplet volume concentration
  - Dry aerosol concentration and particle size distribution
  - Volume mean diameter of dry aerosols and of water droplets.

The ISP with the idealized conditions (single room geometry, steady state thermal hydraulics) gives a good picture of both the capability of the codes and the users as well and of the quality
of the experimental test facility. The agreement of the results with the measurements was not as good as expected. In particular the aerosol condensation modelling and the accuracy of related thermal hydraulic parameters should be improved.

− The solubility effect increases the growth of hygroscopic particles by condensation and enhances the aerosol depletion. An appropriate modelling is absolutely necessary. The solubility model in MELCOR needs some corrections.

− The Kelvin-effect may slow down the depletion of insoluble and slightly soluble aerosols in a condensing atmosphere. There are indications that the Kelvin-effect is not treated well by all codes except ASTEC and COCOSYS. The modelling of the Kelvin-effect should be checked.

The multi-component aerosol behaviour in the KAEVER tests was fairly easy to calculate, because the components were well distributed among all particles. Experiments with partly mixed aerosol components are needed to validate the multi-component capability of codes. For the calculations with a correct aerosol condensation treatment the largest discrepancies in the aerosol results were caused by the uncertain thermal hydraulic variables "relative humidity" and "volume condensation rate".

Furthermore, uncertainties of the initial and boundary conditions and of some measured parameters (e.g. aerosol injection rate) explain to a certain extent the spread of the consistent analytical results. The user influence on the aerosol results is high for the MELCOR-calculations of five participants. It is mainly caused by problems with the solubility model and the different attempts to overcome them. Without these attempts the droplet growth and the aerosol depletion was overestimated considerably.

ISP44 shows quite a large user influence on the results. Possible measures to reduce this influence are the improvement of code input assistance, user training, further benchmarks etc.. In the ISP37 on test VANAM M3 all codes were already used except the new ones ASTEC and COCOSYS. The exercise comprised the depletion of a strongly hygroscopic aerosol in a multi-compartment geometry and was more complex than ISP44. Among the most uncertain variables and models analyzed were already "volume condensation rate", "relative humidity" and the
solubility model. This demonstrates the necessity to perform several exercises on an important topic within a certain time.

Aerosol depletion in a condensing atmosphere is quite well understood and the models used are valuable tools for real plant applications. The situation in real plants however is more complex especially the geometry, the expected thermal hydraulic transient and the aerosol generation and release. In addition there are other important phenomena, e.g. dry and wet resuspension, the multi-compartment fission product behaviour, aerosol removal by pool scrubbing and sprays, etc., which have to be taken into account.

The outcome and the experiences gained with ISP44 were a very valuable contribution to the discussions about the state of knowledge in aerosol physics and behaviour. They will be very helpful in preparing the State-of-the-Art Report on Nuclear Aerosols in Reactor Safety.
1 Introduction

A standard problem is defined as a comparison between experimental and analytical results, in this case out of the field of reactor safety research. The detailed comparison of the data permits conclusions for the reliability and precision of computer simulations of postulated accidents and contributes to the development and improvement of reactor safety computer codes [1].

Following a suggestion of the Federal Republic of Germany, the OECD-CSNI\(^3\) agreed on its 1998 December meeting to offer experiments from the KAEVER test series [2], performed at Battelle GmbH, Eschborn, Germany as International Standard Problem No. 44 (ISP44) to its member countries\(^4\). The experiment and the execution of the ISP are sponsored by the German Federal Ministry of Education and Research and by the German Federal Ministry of Economics and Technology, respectively. The ISP will be conducted as a "blind" standard problem, i.e. besides initial and boundary conditions, the relevant experimental results have been locked and not delivered to the participants in the ISP prior to performing the calculation. Similar test results of the KAEVER test series are available to the participants for “open” calculations.

After the preparatory meeting [3], held at Gesellschaft für Anlagen- und Reaktorsicherheit (GRS) mbH, Köln, Germany on January 25 and 26, 2000, 10 organizations from 9 countries submitted their results for comparison and evaluation.

ISP44 follows a series of former ISP in this area. The most related ones are ISP37 (VANAM M3 Aerosol Behavior in the Battelle Model Containment) [4], AHMED Code Comparison Exercise [5], and CEC benchmark problems (Benchmark on FIPLOC Verification Experiment F2: Thermal-Hydraulics in the Battelle Model Containment BMC and Benchmark on DEMONA B3 Experiment: Thermal-Hydraulics and Aerosol in the BMC) [6, 7].

\(^3\) Organization for Economic Cooperation and Development - Committee on the Safety of Nuclear Installations

\(^4\) As it has already been done in previous ISP, non-OECD countries are invited to participate, too
2 Objectives of the Standard Problem

During an unmitigated severe LWR accident with core melt-down, radioactive fission and activation products are being released into the containment as gas, vapor or, to a great extent, adsorbed on aerosols, while the containment building serves as a final barrier to the environment. Since the time dependence and distribution of fission products and aerosols are very important to mitigate the accident, e.g. by venting, a detailed knowledge of fission products and aerosols behavior and a relevant analytical prediction capability is of great importance. Experimental results and code predictions can be used to quantify the safety margins presently existing in the safety systems of operating reactors, and to explore possibilities of mitigating the severe accident consequences. For demonstrating the capability of current computer codes to model and to calculate the aerosol distribution and settlement in a containment with sufficient accuracy, the OECD-CSNI decided to propose a containment aerosol behavior standard problem.

The general objectives of the International Standard Problem No. 44 (ISP44) are to analyze the aerosol behavior, e.g. volume condensation and settlement of aerosols in a containment atmosphere with well defined thermal-hydraulic boundary conditions.

In more detail the objectives of ISP44 are the comparison and investigation of the following physical variables and phenomena:

- State-of-the-art status review on computer codes for containment analysis, e.g. aerosol behavior and partly, thermal-hydraulics

- Phenomena and physical variables to be investigated:
  - Pressure in the test vessel
  - Atmospheric temperature in the test vessel and the vessel sump area
  - Wall temperatures inner and outer test vessel (insulated) and inner and outer doorway (not insulated)
- Relative humidity
- Volume condensation rate
- Dry aerosol concentration
- Volume mean diameter of dry aerosols
- Water droplet volume concentration
- Volume mean diameter of water droplets
- Particle size distribution
- etc.

3 Description of the test facility

3.1 Vessel Design

The KAEVER test facility is a former 1:1 test mockup for a nuclear reactor containment personnel airlock. It is a horizontal cylindrical steel vessel with plane faces, where short doorways are attached on both sides. The overall shape is shown in Figure 3.1.

Parts of the vessel walls are thermally insulated, as indicated in the figure. Parts of the insulated surfaces are equipped with electric heater mats. The doorway fronts (surface parts 7*) have doors that can be operated by an opening mechanism. In Figure 3.2 and Figure 3.3, the vessel dimensions are indicated. Dimensions in the figures are given in mm.

Some external components of the test vessel like the support structure or the opening mechanisms of the doors are also indicated in Figure 3.2 and Figure 3.3. These components participate in the heat transfer from the vessel to the ambient.

The vessel has an inner free volume of 10.595 m$^3$. During condensation of steam, the condensate accumulates on the bottom of the cylindrical part, but the sump level of the cylindrical part does not reach the elevated floors of the doorways. The contact area between sump water and cylinder wall rises with increasing sump water mass.
The doors provide an easy access to the vessel interior. Repeated opening and closing of the doors may be a reason why the leakage of the vessel slightly varies between different experiments.

3.2 Heat Conducting Walls

The walls of the test vessel are made from steel. Most parts of the outer surfaces, including the doorways and the doors, carry an outer thermal insulation layer. Most of the insulated outer surfaces are also equipped with electric resistance heater mats between the steel wall and the insulating layer, as indicated in Figure 3.1. Uninsulated parts of the doorways are associated with the opening mechanisms of the doors, where it was not possible to provide a suitable insulation. These parts form the major heat transfer path to the environment during experiments with heated vessel. Furthermore, the opening mechanism has a large mass of steel that is in contact with the vessel wall, and represents another path for heat losses.

The outer edge of the insulation layer carries an additional steel layer of 2 mm thickness. Heat losses from the vessel to the environment are also associated with heat conduction to massive structures present in the door opening mechanisms and the vessel support structures. Since these heat transfer paths are difficult to be quantified, special heating tests were performed where additional temperatures at the outer surfaces were measured. These tests were analyzed to determine effective areas and thicknesses for parts of the vessel wall suitable for thermal hydraulic model simulations.

3.3 Thermal Hydraulics

Thermal hydraulic conditions inside the vessel are generally well mixed. The thermal gradients introduced by the uninsulated wall parts lead to a natural convection loop which mixes the vessel atmosphere within several minutes. The steam injection occurs near the vessel bottom which also promotes mixing.

The thermal-hydraulic behaviour is determined by the operation of the electric heater elements, the injections, the heat losses and the leakage. Injections of steam and nitrogen are provided. Carrier gas for the aerosol injection and cleaning gas for the photometer tubes is also nitrogen. Sampling from the atmosphere is carried out as controlled withdrawal of the steam/gas/aerosol
mixture over an aerosol filter and a cooling device, where the steam is condensed; the non-condensable gas flow is then determined. Sump water can be drained at the bottom. The electric heater system is temperature-controlled.

### 3.4 Aerosol Injection and Deposition

The aerosol injection is established by inductive heating of 1 or 2 crucibles until evaporation of the materials in the crucibles occurs, and a nitrogen carrier gas flow to transport the condensation aerosols from the crucibles into the test vessel. The carrier gas flow rate is monitored continuously. Filter samples from the aerosol injection line are taken at several times and analyzed for concentration and size distribution.

Surface areas for aerosol deposition are the vessel walls, the sump water surface, and the surfaces of the built-in instrumentation, the latter being a negligible fraction of the total deposition surface.

### 3.5 Instrumentation

The locations of measurement transducers are indicated in Figure 3.4. The figure also indicates the positions of injection ports and sampling lines.

The thermal hydraulic instrumentation is based on sensors for pressure (P sensors), atmospheric and wall temperature (T sensors) and relative humidity (HK sensors). Additional sensors are provided to measure the flow rates of injected steam and nitrogen, the electric power of the heater mats and the water consumption of the steam generator.

The main aerosol instrumentation consists of:

- sampling lines (PN positions) for withdrawal of atmospheric fluid over an aerosol filter. The evaluated filter data give concentrations and size distributions of dry particle mass in the atmosphere. Size distributions are also derived from impactor samples.

- spectral extinction photometer (PHM) measurements with 12 different spectral wavelengths. The evaluated data give concentrations and size distributions of droplets in the atmosphere.
The aerosol release from the crucibles is controlled by pyrometers to determine the temperature at the outer sides of the crucibles, and a conventional photometer to get a qualitative indication of the development of aerosol smoke. When mixtures of 2 materials are evaporated together in a single crucible (Ag and CsI), the temperature levels shown by the pyrometer signal are correlated with the boiling points of the material components, and the more volatile material (CsI) is evaporated first.

For some experiments with mixed aerosols, a limited number of aerosol filter samples were chemically analyzed to determine the material composition.

### 3.6 Accuracy of Measurements

The technical error bands of the transducer systems are:

- **Pressure**: ± 0.01 bar
- **Temperature**: ± 1.2 °K
- **Relative humidity**: ± 10 %
- **Gas flow rates**: ± 0.2 l/min
- **Steam flow rate**: ± 0.15 g/s
- **Heating rate**: ± 30 W

When the humidity sensor is in contact with a wet atmosphere, the transducer signal rises to a value around 110 % which is outside the measuring range. This signal can only be used as an indication of atmospheric saturation (100 %). Values below 100 % have a physical meaning. However, a closer inspection of the time dependent signals indicates that even under superheated conditions the data are not quantitatively corresponding to the actual conditions in the vessel. Therefore, the humidity measurements are only considered qualitatively to distinguish between saturated and superheated states.
4 Description of the Experiments

4.1 Experimental Procedure

The general procedure for an experiment includes the following steps:

Phase I: Preconditioning of the test vessel

During this phase, the vessel is flushed with steam, and the electric heating is applied to reach elevated wall temperatures. The data acquisition system is not operated. The preconditioning is continued until quasi-stationary conditions are obtained. At the end, withdrawal of sump water concludes the preconditioning phase.

Phase II: Execution of the aerosol experiment

The thermal-hydraulic conditions in the vessel are readjusted by controlled steam injection and electric heating, in order to reach a quasi-stationary state that may differ from the final state of phase I. Then, aerosols are injected by turning on the inductive heating of the aerosol generators until the material in the crucibles is completely evaporated. Finally, the depletion of aerosols is observed without further change in the injection or boundary conditions.

According to the aims of the particular experiment under consideration, details can differ from this general procedure.

4.2 Choice of ISP Experiments

The following KAEVER experiments are subject of the ISP 44:

- **K148**: test with Ag aerosol
- **K123**: test with CsI aerosol
- **K188**: test with CsOH aerosol
- **K186**: test with mixed aerosol of Ag and CsOH
- **K187**: test with mixed aerosol of Ag, CsOH and CsI (blind calculation)
The hygroscopicity of the materials increases from the insoluble Ag over CsI to the very hygroscopic CsOH. Thermal hydraulic conditions applied during the tests are generally at 100% relative humidity with a limited degree of supersaturation, resulting from steam injection into the preheated test vessel. The most important variation parameter in this selection of tests is the hygroscopic effect associated with the aerosol material, and its impact on the aerosol sedimentation rates.

The experimental data taken during phase II covered different time ranges in the various experiments considered for the ISP44. The readjustment phase before the aerosol injection lasts between 10 minutes and 6 hours. The aerosol injection phase takes ½ to 2 hours, and the subsequent observation of aerosol depletion takes a time span between 3 ½ to 4 ½ hours.

4.3 Selected Experimental Results

The experimental pressure measurements of the selected tests are shown in Figure 4.1. The time axis is normalized in this figure to begin with t=0 at the start of the aerosol injection. The pressure increase is caused by the injection of nitrogen carrier gas during the aerosol injection period. The variation in the pressure levels between 2.3 bar and 3.4 bar after the end of the aerosol injection is related to the length of this injection phase.

The atmospheric temperatures are shown for test K186 as an example in Figure 4.2. This figure has the time axis origin according to the original data; aerosol injection starts at time 10 minutes and lasts for 2 hours. The highest temperature in the figure T9.1 is in the centre of the vessel. A similar temperature level is reached by T10.3 at the inner cylinder wall. T10.1 and T10.2 are inner and outer wall temperatures at the uninsulated wall of the doorway. T9.2 is a sensor near the bottom of the test vessel. Comparison of T9.1 and T9.2 indicates some thermal stratification.

The relative humidity sensor shows values above 100% for all times in test K186.

Time-dependent aerosol injection rates were estimated from the available data by the following method. From the measured aerosol mass concentration in the vessel, the total aerosol mass release rate was calculated by numerical differentiation with respect to time, assuming a constant aerosol depletion rate. The injection rates of the individual aerosol material components were then approximated by Gaussian profiles, where the location and width on the time axis were determined from the pyrometer and photometer data, and the intensity adjusted according
to the measured mass inventories in the crucibles. A final adjustment of the rates was done with the help of numerical simulations using FIPLOC and comparison with the measured aerosol concentration transient in the vessel. As an example, the aerosol injection rates for K186 are shown in Figure 4.3.

A comparison of the measured aerosol concentrations is shown in Figure 4.4. The time axis is normalized in this figure to begin with t=0 at the start of the aerosol injection. The most important results from this figure are the differences in the aerosol depletion rates. The smallest rate is given for the non-hygroscopic material Ag in test K148. The CsI test K123 shows an intermediate depletion rate. The pure CsOH test K188 has the highest rate, and the rates in the mixture tests K186 and K187 are only slightly smaller. The depletion rate is clearly dominated by the most hygroscopic component, since this determines the amount of water attached to the aerosol particles.

Droplet concentration data for K123 from the spectral photometer are shown in Figure 4.5. Between 4.2 and 5 h, droplet concentrations are too high such that no reliable signal could be evaluated. The average droplet and dry particle diameters are given in Figure 4.6, showing the consistency of the photometer and the impactor measurements.

In Figure 4.7 the droplet size distribution for test K186 at a time of 1000 s after the end of the aerosol injection is shown, as determined by the spectral photometer. Data refer to size-class specific droplet concentrations.

5 Calculations by the Participants

5.1 Participants and Codes

Representatives of 10 organizations from 9 countries participated in the International Standard Problem No. 44 (ISP44) based on the KAEVER experiment on the behavior of core-melt aerosols in a LWR containment. They submitted 10 contributions [8 to 17] using the codes ASTEC-V0.3, COCOSYS V1.2, CONTAIN 2.0, MELCOR 1.8.3, 1.8.4, 1.8.5 and ART MOD2/REMOVAL [18 to 22]. All participants delivered results for the “blind case”, and with one exception (NRI) for the “open” cases. Table 5.1 summarizes the participating organizations, the calculated cases and the codes used. All codes use lumped parameter assumptions.
### Table 5.1: Participants and Codes Used

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<thead>
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<th>Organization</th>
<th>Author</th>
<th>Legend</th>
<th>Code</th>
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<td>GRS/IPSN</td>
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<td>Jozef Stefan-Institute</td>
<td>I. Kljenak, B. Mavko</td>
<td>IJS</td>
<td>CONTAIN 2.0</td>
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<td>VEIKI</td>
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5.2 Selection of Variables to be Calculated

The selection of variables to be calculated by the participants was done in order to meet the objectives of the ISP. Special attention was given to the correct representation of the overall thermal hydraulic and aerosol behavior of the containment model, to suitable location of a measurement device and to an acceptable measurement error. Only those variables which meet these criteria have been chosen for comparison.

The main thermal hydraulic variables are pressure and temperature. Due to relatively large measurement errors for the humidity and heat transfer to the structures only general results are given.

The selected aerosol variables are aerosol and airborne water concentration, geometric standard deviation and particle size distribution.

A detailed list of all variables is given in the specification of ISP44 [23].

5.3 Codes and Computational Models Used for ISP44 Calculations

5.3.1 General Code Descriptions

The following part contains short general code descriptions as far as available from the participants.

CONTAIN

CONTAIN has been developed by the Sandia National Laboratories and is the US Nuclear Regulatory Commission's principal best-estimate, mechanistic containment analysis tool for severe accidents [20]. CONTAIN is an integrated analysis tool used for predicting the physical, chemical, and radiological conditions inside a containment building following the release of radioactive material from the primary system. The interactions among thermal hydraulic phenomena, aerosol behavior and fission product behavior are taken into account. The code includes atmospheric models for steam/air thermal-hydraulics, intercell flows, condensation/evaporation on structures and aerosols, aerosol behavior, fission product transport, effect of
fission product decay, and gas combustion. It also includes models for reactor cavity phenomena such as core-concrete interactions and coolant pool scrubbing.

**MELCOR**

The code MELCOR is being developed by the Sandia National Laboratories for the US Nuclear Regulatory Commission [21]. It is a fully integrated, engineering-level computer code that models the progression of severe accidents in LWR nuclear power plants. A spectrum of severe accident phenomena, including reactor coolant system and containment thermal hydraulic response, core heat up, degradation and relocation, and fission product release and transport, is treated in MELCOR in a unified framework for both boiling water reactors and pressurized water reactors.

**ASTEC**

The French-German integral code ASTEC (Accident Source Term Evaluation Code) [18] is being developed by IPSN (Institut de Protection et de Sûreté Nucléaire), France, and GRS (Gesellschaft für Anlagen- und Reaktorsicherheit), Germany, since 1994. The first version (ASTEC V0), already released to several European organizations, has been based on the best models of the French integral code ESCADRE and on the German containment codes RALOC for thermal-hydraulics and FIPLOC for aerosol behaviour (the main models in the latter code were based on the MAEROS code, developed by Sandia National Laboratories, USA).

Only the ASTEC module CPA was activated in the calculation of the KAEVER tests: it describes thermal-hydraulics and aerosol behaviour in the containment.

The module CPA is a “lumped-parameter” or “multi-zone” code. It consists of a thermal-hydraulic part (CPA-THY) and an aerosol and fission product part (CPA-AFP).

1. **CPA-THY**

In this exercise only a small part of the thermal-hydraulic capabilities was used:

- pressure and temperature build up and history,
- energy distribution, heat transfer and heat conduction in structures.
For the KAEVER simulations the most important variables are the bulk condensation rate and the atmospheric humidity.

2. 

CPA-AFP

The aerosol model describes the behaviour of a homogeneously mixed polydispersed aerosol system inside a control volume. The system may be composed of up to 8 chemically different aerosol components. Agglomeration, condensation, deposition and existing aerosol sources (injections) and sinks (aerosol discharges) are calculated. The particle size range is discretised by a maximum of 20 particle size categories. Each size category may be differently composed of the various chemical components. However, within each category a homogenisation will be performed so that all particles of one given category will have the same component composition.

COCOSYS

The COCOSYS system [19] provides a tool based on mechanistic models for the simulation of essential processes and states during severe accident propagation in the containment of nuclear power plants. The complete system is subdivided into several so-called main modules. Each main module is a separate executable program used for specified topics of the whole process. Between these main modules, the communication is realised via a driver program using PVM (parallel virtual machine). The separation into different main modules considers that the strongest coupling between the main modules is on the time step level to avoid a high-frequency data transfer. The amount of data transferred is relatively small, due to a suitable distribution of the complete topology and topics of the systems to the different main modules. For future COCOSYS versions, this concept will be extended to realise parallelism on the main module level.

The compartments of the NPP under consideration (or other building types) have to be subdivided into control volumes (zones). The thermodynamic state of a zone is defined by its temperature(s) and masses of the specified components (lumped-parameter-concept). To realise more complex boundary conditions or processes, a flexible program and data structure is installed. For example, each zone can be split into several so-called zone parts. The thermal hydraulic main module contains different kinds of zone models, like non-equilibrium zone model and or a zone model simulating hydrogen deflagration. For a realistic simulation of severe accident propagation, a detailed modelling of the safety systems is important. The THY (thermal hydraulic) main module can simulate coolers (including intermediate cooling circuits), spray
systems, fan and air conditioning systems, ice condensers and catalytic recombiner systems. The developed pyrolysis models are implemented inside the THY main module.

The COCOSYS aerosol-fission-product (AFP) main module is used for best-estimate simulations of the fission product behaviour in the containment of LWR (light water reactors). Both, the thermal hydraulic (THY) and the aerosol-fission-product (AFP) main module consider the interactions between the thermal hydraulics and aerosol fission product behaviour. Particularly for hygroscopic aerosols, a very tightly coupled feedback on the thermal hydraulics (especially for the saturation degree) can be considered. AFP can calculate up to eight different aerosol components, with their own chemical characteristics and size distribution.

The FIPHOST module calculates the transport of fission products carried by so-called hosts (carrier for fission products) in the containment. The mobile hosts are gas, aerosol and water, the immobile hosts are the surfaces in atmospheric and sump spaces. All the relevant transfer processes of the fission products between hosts are modelled: aerosol depletion by natural processes and by engineered systems like filters, recombiners or spray systems, wash-down from walls into sumps, etc. Host changes as a consequence of chemical reactions or the decay of radioactive isotopes are also taken into consideration.

**ART/MOD2 - REMOVAL**

The ART/MOD2 – REMOVAL codes [22], developed by JAERI, calculate only the aerosol behaviour.

ART Mod2 analyzes the behavior of Fission Products (FP) in reactor coolant system and containment during LWR severe accidents. The code can consider FP removal by natural deposition and by engineered safety features such as spray systems. As for the FP aerosol deposition, the code can treat gravitational settling, thermophoresis, diffusiophoresis, Brownian diffusion and resuspension. Concerning the gaseous FP, the code can deal with condensation, chemisorption and revaporization. The code also considers the aerosol growth by gravitational, Brownian and turbulent agglomeration and condensation or revaporization of gaseous FP at the aerosol surface.

For hygroscopicity in REMOVAL model, Mason’s equation is used to calculate aerosol growth by steam condensation. To calculate aerosol growth due to hygroscopicity, the relative humidity at
aerosol surface in Mason’s equation is reevaluated taking into account the Kelvin’s effect and the Raoult’s law. Then, the equilibrium aerosol size is calculated by iteration until the growth rate becomes zero. Since it usually takes much CPU time for iteration calculation, the equilibrium radius of aerosol is calculated by assuming the aerosol surface temperature equal to atmospheric temperature and the value is used during the iteration to reduce computation time.

5.3.2 Computational Models Used by the Participants

The following code options and modeling features as far as they are relevant in this ISP and delivered by the participants are discussed here [8 to 17]:

- coupling between atmosphere and water,
- flow equation,
- maximum water content in a node and drainage,
- sump simulation,
- heat transfer

CONTAIN

An atmospheric node can contain water as airborne droplets and condensate film on the wall. When the film thickness exceeds a limiting value, water is drained into a specified sump. Optionally a film tracking model can be used.

The atmosphere is in thermal equilibrium with the airborne water, but the water film can have a lower temperature (non-equilibrium).

Pool or sumps can be modeled by a specific option, which simulates the pool with an atmospheric layer above and a structure with a fixed temperature boundary at the bottom. Heat and mass exchange (condensation and evaporation) is calculated between the pool and the atmosphere.

The CONTAIN flow equation is similar to the one used in FIPLOC.
Within the CONTAIN code the aerosol behavior is simulated by the aerosol model MAEROS. Several enhancements to the original MAEROS have been added applying aerosol processes in a LWR-containment.

MAEROS is a multi-component aerosol code which evaluates the dynamic particle size distribution of each component in a control volume. The distribution is discretised in a number of particle size classes (sections). All particles within a section have the same composition including the water condensed on the particles. The most important constraint is that the material density is assumed to be the same for all components including the airborne water.

In MAEROS four agglomeration processes are treated: Brownian diffusion, differential gravitational settling, turbulent shear agglomeration, and turbulent inertial agglomeration.

Four natural deposition processes are modeled: sedimentation, diffusion to surfaces, thermophoresis, and diffusiophoresis.

Condensation or evaporation of water on/from the aerosol is calculated either by the fixed grid or the moving grid technique. With the fixed grid technique the Mason equation is solved in a common time step together with the agglomeration and depletion processes. Kelvin and solubility effect are not considered.

By use of the moving grid model MGA the calculations of the particle growth or shrinking by condensation and evaporation respectively are separated from the other aerosol processes. The algorithm is based on the methods of characteristics to calculate the trajectories of the sectional boundaries. The Mason equation is used including the Kelvin and the solubility effects. After each MGA time step the aerosol are remapped onto the MAEROS fixed grid again. In the proceeding MAEROS time step the water component is treated like a solid component. In CONTAIN the fixed grid and the moving grid method are available.

In multi-component geometries the airborne particles are transported by the atmosphere flows between the control volumes.


MELCOR

When equilibrium thermodynamics is used in a control volume, mass and energy transfer between the pool and the atmosphere is implicitly determined by the assumption that the pool and the atmosphere are in thermal and evaporative equilibrium.

If a volume, in which non-equilibrium thermodynamics is specified, contains both a pool and an atmosphere, the mass and energy transfer between both is calculated by condensation, convection and evaporation.

The flow equation simulates two phase flow (atmosphere and water), e.g. atmospheric flow and drainage are simulated with the same equation in the same flow path. Similar to the codes above the derivative of the velocities in respect to time is calculated using the buoyancy term, the pressure balancing term and the unrecoverable pressure loss. But in addition the following terms are simulated:

- momentum through the flow path by area changes
- interface force between atmosphere and water

The following flow regimes are possible:

- pure atmospheric flow
- two phase flow, same direction or counter current
- pure liquid flow

In MELCOR the aerosol behavior is calculated by the MAEROS model, but without direct inclusion of condensation and evaporation in the MAEROS solution framework.

The particle growth/shrinking by steam condensation/evaporation is calculated separately by the Control Volume Hydrodynamics (CVH) package. Water droplets are transported as fog by the CVH package and treated as water-class aerosols by the RN package. The difference between CVH fog and RN water-class masses in a control volume at the end of the CVH time step represents net condensation of water onto or evaporation from the aerosol in that volume. The net change in the water mass is imposed on the water-class inventory in the RN package, which
then uses the Mason equation to distribute the mass over the aerosol size distribution in the control volume.

Beside the originally implemented conventional Runge-Kutta integration routine an explicit (forward Euler solver) is used to increase the efficiency.

The aerosols are transported between the control volumes by the flow of atmosphere and pool water, assuming zero slip between the aerosol and the host medium. Additionally in absence of bulk flow, aerosols may move by Brownian motion or by gravitational settling through openings between control volumes.

**ASTEC**

**- Agglomeration processes**

The process referred to as agglomeration or coagulation describes what happens when two or more particles collide, stick to each other and form a larger particle. The agglomeration rate rises quadratically with the particle number concentration. In LWR containment, agglomeration rates can be expected from about 1 g/m$^3$ aerosol concentration. Four different aerosol processes are modelled (here the two first processes are dominant):

- Brownian agglomeration,
- gravitation agglomeration,
- turbulent shear agglomeration,
- turbulent inertial agglomeration.

Brownian agglomeration takes place through the Brownian movement of aerosol particles in the gas. It is the dominating effect in containment. It is proportional to the agglomeration form factor $\chi$ and reverse proportional to the dynamic form factor $\gamma$. With these factors, the deviation of the particles from the spherical form is taken into account. For spherical particles $\gamma = \chi = 1$.

The gravitational agglomeration takes into account the collision of large, faster falling particles with smaller and thus slower ones. The collision efficiency $\varepsilon$ for the gravitational agglomeration indicates the probability with which particles that collide will actually stick to each other. Different relations for $\varepsilon$ are available in CPA-AFP: Fuchs relation, Pruppacher-Klett one and the original MAEROS one. The agglomeration rate increases with growing collision efficiency and increasing agglomeration form factor. It decreases with increasing dynamic form factor.
- **Deposition processes**

The aerosol model takes the following deposition processes into account:

- sedimentation,
- diffusive deposition,
- thermophoresis,
- diffusiophoresis.

Like the agglomeration coefficients, the deposition coefficients are not calculated anew for each time interval but are determined from a table of coefficients drawn up at the start of the calculations by interpolation in line with the overall pressure and the temperature. Sedimentation is the deposition of particles on floor surfaces by gravity. As the sedimentation process in a well-mixed volume takes place in a thin boundary layer along the surface, all horizontal surfaces serve as sedimentation surfaces. In LWR containment, sedimentation is generally the most effective deposition process.

Separation through diffusion takes place as Brownian movement in the concentration gradient on the surface. It is mainly relevant for small particles. The user must provide the boundary layer thickness. Thermal-hydraulic separation of aerosol particles takes place in the temperature gradient of a boundary layer on a cold wall. In LWR containment it only plays a subordinate role since there are no great temperature differences between the dry atmosphere and the wall. The aerosol model uses an empiric value of 3 mm for the thermophoretic boundary layer thickness. Diffusiophoretic deposition takes place through steam condensation on a cold wall caused by the aerodynamic Stefan flow.

- **Condensation method MGA**

Condensation on the particles is calculated with the moving-grid-method MGA. It reduces calculation times and the numeric diffusion compared to the fixed-grid method. The moving-grid method to calculate condensation on particles was developed by F. Gelbard (Sandia National Laboratories, USA). During the calculation, the grid of the particle size categories is apparently moved. In the case of the conventional fixed-grid method, growing particles are passing through the grid. The thermal-hydraulic model (CPA-THY) and the aerosol models (CPA-AFP) have their own time integration in the program system and are closely coupled to each other. During the condensation interval, the thermal-hydraulic boundary conditions remain constant. They are only
updated before the next interval. However, MGA is internally performing a simplified thermal-hydraulic calculation. In the aerosol interval that follows, the wet aerosol is treated like a dry one. Agglomeration and deposition of the droplets are calculated as if they were solid particles, i.e. the amount of airborne water and its distribution to the solid particles is not altered. In the MGA method, the particle growth and particle shrinking rate are given by the Mason equation.

With the surface tension, the influence of the Kelvin effect on the particle growth is taken into account. The Kelvin effect depends strongly on the particle size. The hygroscopic effect is described in the equation by the chemical activity of the solution, which is determined by the Vant’Hoff factor. It corresponds to the number of ions into which a molecule of the salt dissociates in an ideal solution (e.g. $a_w = 2$ for NaOH). For insoluble substances, $a_w = 0$. In MGA the assumption is that there is always an ideal solution present in which the chemical activity decreases at an increasing molar proportion of the water in a droplet.

**COCOSYS**

The compartments of the KAEVER test facility are subdivided into control volumes (zones). The thermodynamic state of a zone is defined by its temperature(s) and masses of the specified components. A zone part can be mainly gaseous, liquid or solid. Gaseous zone parts may contain liquid or solid particles (fog or dust), liquid zone parts may contain dissolved gases and solid particles and solid zone parts may contain dissolved gases and liquids. Five different zone models are implemented in COCOSYS whereas two zone models are important to simulate the KAEVER test facility.

The first of them is the more simple “equilibrium” zone model is representing the environment. All components (liquid water, vapour and other non-condensable gases) are assumed to be mixed homogeneously, resulting in a homogeneously distributed temperature in the control volume (only one value). Superheated as well as saturated conditions are considered. Superheated atmospheres cannot contain liquid water. In these cases the water is drained immediately into other zones. Using the concept of sump zones a quasi non-equilibrium behaviour can be simulated. The volume of the environment zone is modelled very large ($0.1E+06 \text{ m}^3$) to prevent physical and numerical problems.

The test vessel is represented by a “non-equilibrium” lumped parameter volume that is connected to the environment by a junction. Using this model the zone is subdivided into two
parts: the atmosphere part similar to the equilibrium zone model and a sump part (if existing) specified by the temperature and water mass. Between both parts heat exchange by convection and condensation (or evaporation) correlation is possible. The volume is set to 10.595 m³ as given in the ISP 44 specification.

Inside of the both modeled zones no internal flows are calculated. A mass flow is only possible between the vessel zone and the environment zone via junction or in the preheating phase via a valve representing the open blind cap. For the main experiment only the loss junction is interesting. This junction is modeled as an atmospheric junction whereas the flow is calculated by an incompressible steady state momentum equation.

The drainage from condensed water into the sump is related to the defined walls. For the KAEVER experiments the heat structures are defined as given in the ISP 44 specification and connected on the first side to the test vessel and on the second side to the environment. The maximum water content in the sump is the whole volume of the test vessel (hypothetical, if the modeled test vessel is completely flooded). The water is removed from the sump by a removal table (in cases with water removal in the ISP 44 specification) only in the preheating phase.

All mass injections and removals in the test phase were defined as given in the ISP 44 specification. They are delivered to the code as an input table. The injections are made directly into the test vessel without consideration of momentum.

Heat transfer is calculated by the code for the surface of the sump and on both sides of the heat structures. In the case of the surface of the sump, the heat transfer can not be chosen and is calculated by the non-equilibrium zone model. Different options can be chosen for the walls. Inside the vessel free convection, forced convection, condensation and wall-gas radiation are calculated. On the outer surfaces free convection, forced convection and wall-gas-wall radiation to surrounding building walls are computed.

The aerosols behaviour is calculated by MAEROS. In the case of presence of aerosols the volume condensation is calculated by MGA. Without aerosols, volume condensation is calculated internally by the non-equilibrium model and no fog formation can appear.
5.3.3 Modeling Information Provided by the Participants

Studsvik

The MELCOR code package is designed in a modular structure with interfaces between them with emphasis on analyses of severe accident in light water reactors. Information between the modules can be considered at each time-step.

The present model for the ISP44 analyze have the following module packages been used: the Control Volume Hydrodynamics package (CVH) for the calculation of the thermal hydraulic conditions within the containment, the Heat Structural package (HS) handle the heat interaction with structural material and finally the Radionuclide Package (RN) for modeling the injection of aerosols and their condensation and deposition on structural surfaces.

In addition the Material Properties package (MP) is used to define the material properties according to the specification given, which then will be used by the HS-packages.

In this study the injection and removal of gases and vapor are treated with Control Functions (CF) within the CVH-package.

List of aerosol deposition surface areas

All the surfaces of heat structures are considered as deposition areas se below the nodalisation. By default, in MELCOR, the heat structures and their orientations as walls and floors are treated as deposition areas as long as no other specifications are given.

Nodalisation and input data

The containment is treated as one volume. In MELCOR the volume is defined by a table with altitude and volume. In the present study the containment is divided in 20 levels and volumes which were approximated to correspond to the volume of the cylinder and the volumes of the door entrances. Around the containment was assumed a room of 1000 m$^3$ with height 10 m, furtheron called environment.

In MELCOR cylindrical heat structures are available, for the main cylinder of the containment this was used, which merge the proposed heat structures 1, 4 and part of 7. The remaining heat
structures are based on data from table D1 in the specification. Some of the recommended heat structures were divided according to this table. The recommended "dummy" heat structure for remaining structures were included, the area of this structure had to be set to 11 m$^2$ to fulfill the hydrodynamic conditions within the containment.

The junction between two or several nodes is in MELCOR treated with the flow package (FL). In this study the leakage from the containment to the environment could be described with such a junction. However, from the information given in the specification the leakage was treated with a control function according to the expression given as removal of mass and energy from the containment, with the assumption that the leakage would have no effect on the environment.

**Jozef Stefan Institute**

**Test Vessel**

The test vessel was modeled as suggested in the ISP44 specification. The internal volume of the vessel is 10.595 m$^3$. The vessel was modeled as a single CONTAIN "cell", whereas the environment was modeled as another cell. As CONTAIN is a lumped parameter code, a simple geometrical configuration was used to model the vessel. The following Table 5.2 provides internal horizontal cross-sections of the test vessel cell between different vertical levels.

<table>
<thead>
<tr>
<th>Elevation range [m]</th>
<th>Cross sectional area [m$^2$]</th>
</tr>
</thead>
<tbody>
<tr>
<td>0 - 0.0535</td>
<td>2.0</td>
</tr>
<tr>
<td>0.0535 - 2.090</td>
<td>5.150</td>
</tr>
</tbody>
</table>

Heat structures were modeled as indicated in the specification.

The surface of the heat structure "wall part no. 10" (see [23]) was set to 8.0 m$^2$.

The heat structure "wall part no. 4" (see [23]) was divided in two parts. One part was modeled as a CONTAIN "lower cell". The area of this part was 2.0 m$^2$, as this is the maximum contact area between the liquid pool and the atmosphere. Namely, it is specified, that the sump level of the cylindrical part does not reach the elevated floors of the doorways.
The remaining part of wall part no. 4 was modeled as a horizontal slab which is never submerged. Other heat structures are also never submerged.

CONTAIN treats all internal surfaces of heat structures and the lower cell as aerosol deposition surfaces. Areas of deposition surfaces are provided in the following Table 5.3.

<table>
<thead>
<tr>
<th>Surface</th>
<th>Area [m²]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ceiling</td>
<td>5.677</td>
</tr>
<tr>
<td>Vertical walls</td>
<td>26.265</td>
</tr>
<tr>
<td>Floor + pool</td>
<td>5.677</td>
</tr>
</tbody>
</table>

Some walls of the test vessel are equipped with heater mats between the insulation and the inside steel. As CONTAIN does not provide options for explicit modeling of this kind of structure, the following approach was used for test K187 (during this test, walls equipped with heater mats were heated during an initial period).

Walls equipped with heater mats were modeled as two separate heat structures, separated by a "fictive" intermediate cell, and a heat flux was applied to the surfaces exposed to the intermediate cell. The heat flux specified in the input data (ISP44 CD\textsuperscript{5}) was partitioned into a fraction applied to the insulation and a fraction applied to the inside steel. The consistency of this approach was verified by checking that the total heat output from the intermediate cell between the inside steel and the insulation was equal to the heat output calculated from the total heat flux, taking into account the corresponding heated area (all heated walls minus 2.0 m\textsuperscript{2} modeled as lower cell).

The heated mat in the lower cell part no. 4 (2.0 m\textsuperscript{2}) was modeled as an intermediate steel layer of 1 mm thickness with volumetric heat generation.

\textsuperscript{5} The ISP44 CD is part of the specification [23]
As the test vessel was heated only during an initial period (e.g. first 3490 s of the preconditioning phase in test K187), the simulation was carried out in two parts with two distinct input models. During the first part, heated walls were modeled as separate structures. The simulation was then continued with a second input model, in which walls equipped with heater mats were modeled as single structures with steel plating, insulation and inside steel layers. However, this second part was started with conditions calculated at the end of the first part as initial conditions. The following data were thus transferred from the end of the first part and taken as initial conditions for the second part:

- atmosphere pressure and temperature
- gas mole fraction of O\textsubscript{2}, N\textsubscript{2} and steam in vessel atmosphere
- temperature profiles in all heat structures
- water pool mass and temperature
- average temperature of lower cell layers (wall part no. 4 modeled as lower cell)
- mass and temperature of condensate film on walls; the film was introduced as water sources on walls, with temperature equal to the temperature of the nearest node used for modeling of heat conduction.

The leaking mass flow rates were calculated with the value of the flow loss coefficient CFC set to 1.35, which corresponds to the value $\zeta = 2.7$ in the specification.

**Aerosol Modeling**

Aerosol parameters were prescribed in the CONTAIN input model as specified on the ISP44 CD.

The aerosol size range was divided into 20 sections.

The CONTAIN option DROPOUT, which causes liquid water in the atmosphere, which may be injected with the steam, to be dropped instantly on the cell floor, was prescribed in the simulation for consistency with simulation of open KAEVER tests.

In test K187, a mixture of Ag, CsI and CsOH aerosols was present. According to the ISP44 CD, surface tension had to be considered only for Ag aerosols, whereas solubility had to be included only for CsOH and CsI aerosols. However, CONTAIN does not allow separate considerations of
surface tension for separate components. Besides, the calculation stopped due to convergence problems in aerosol calculations if the surface tension was prescribed. Therefore, the simulation was carried out without taking surface tension into account, thus neglecting the Kelvin effect.

The CONTAIN code calculates the mass in dry material and water within each aerosol size class at each time step. The volume median diameter of wet aerosol particles was determined based on the size class boundaries used in the calculation. However, to determine the volume median diameter of dry aerosols, size class boundaries for dry particles were determined at each time step from size class boundaries of wet aerosols and the ratio of volume of water to volume of dry material in each size class at each time step.

As CONTAIN does not allow separate values of density for different components of an aerosol mixture, a weighted averaged density was used, based on the total injected mass of each aerosol component.

**Vapor Condensation on Aerosols**

The aerosol mass in the test vessel atmosphere increases due to vapor condensation on aerosol particles and due to aerosol injection, and decreases due to aerosol deposition. The aerosol injection rate was specified among provided boundary conditions on the ISP44 CD and was included in the CONTAIN input models. Time-dependent aerosol masses in the vessel atmosphere and aerosol deposited masses were obtained from the simulations. The increase of aerosol mass due to condensation between two successive output values was then obtained from a simple mass balance. Finally, the condensation rate was calculated as the increase of aerosol mass due to condensation between successive output times, divided by intermediate time intervals.

**Initial and Boundary Conditions**

Initial and boundary conditions (initial pressure in the test vessel, initial temperature of the atmosphere and heat structures, environment temperature, heat injection, gas injection, liquid removal, aerosol injection) were included in the CONTAIN input model as specified on the ISP44 CD, except for the following parameters in test K187:

- for steam injection during the preconditioning phase, the mass flow rate $2.99 \cdot 10^{-3}$ kg/s was replaced with the value $3.25 \cdot 10^{-3}$ kg/s.
– for gas removal during the preconditioning phase, the mass flow rate \(7.73 \times 10^{-4}\) kg/s was replaced with the value \(12.5 \times 10^{-4}\) kg/s.

The steam injection rate and the gas removal during the preconditioning phase were prescribed as suggested in the ISP44 specifications.

**University of Bochum**

**List of Aerosol Deposition Surface Areas**

All structures were implemented as given in the ISP44 specification. The walls of the surrounding hall were included, also.

**Input data that differ from the specification**

The pre-heating phase (Phase I) was as in the open test cases set to 100,000 seconds (ca. 28 h). The air removal in Phase I was done through an open valve to the environment zone. This procedure gives a more realistic behaviour than an air removal table and also a much better handling of the thermal hydraulic behaviour in Phase I.

An interesting observation was that there is still some air (nitrogen) in the test vessel at the end of Phase I (more than injected by the cleaning gas table).

The calculation of the Kelvin effect was switched off because of the presence of hygroscopic aerosols. Furthermore some calculations including the Kelvin effect were done additionally to prove that the Kelvin effect has not to be taken into account. The simulations were very instable and had to be restarted several times. Only 3/4 of the whole simulation time of Phase II could be calculated. At the end a thermal hydraulic time step of 0.1 s was necessary. Up to that point, no significant differences between the calculation with and without Kelvin effect occurred.

**Description of the analytical model**

**Thermal hydraulic**

– One lumped parameter volume for the test vessel, non-equilibrium sump zone model.

– One lumped parameter volume for the environment, equilibrium zone model.
− Heat structures as given in the specification connected to test vessel and environment.
− One junction as given in the specification representing the mass losses from test vessel into environment.
− One valve junction representing the opening between the test vessel and the environment in Phase I. It is closed 2000 s before the end of Phase I.
− Volume condensation is calculated by MAEROS/MGA.

Aerosol model

− Agglomeration is computed by MAEROS. Agglomeration shape factor is set to 1. Collision efficiency is calculated according to Pruppacher and Klett.
− The aerosol component behaviour is handled by MAEROS.
− Steam condensation/evaporation is calculated by MGA. Component solubility is set as given in the specification, Kelvin effect is switched off.
− Deposition is calculated by MAEROS. Dynamic shape factor is set to 1.
− 20 particle size classes from 0.010 µm to 50.0 µm are computed. Coupling between models as described in the COCOSYS User Manual.

GRS

The test vessel was simulated by a single compartment.

Thermal Hydraulic Model

The non-equilibrium option is used. This means that the sump and the atmosphere are connected by heat and mass transfer. The environment is simulated by a large node.

The heat transfer models inside the vessel are free convection, condensation and wall gas radiation. A characteristic length of 0.05 m is used for K123, K186 and K188. For K148 however the length of 0.05 m resulted in numerical problems related to the Kelvin effect. 1 m is input instead. The characteristic beam length for the radiation is estimated with 0.7 m in all cases.

Outside the vessel free convection and wall gas wall radiation is simulated.
Aerosol Model

Agglomeration

Brownian and gravitational agglomeration are modeled.

The collision efficiency is calculated with the Pruppacher Klett Model.
The agglomeration shape factor is 1.0.

Steam condensation on the aerosol and evaporation from aerosol

The calculation of the volume condensation rates see above.
The solubility effect is simulated when a Van’t Hoff factor is input. The values given in the CD-ROM are used.
The Kelvin effect was simulated only for the case K148.

Deposition

The deposition by sedimentation, diffusional and diffusiophoresis is modeled. The diffusion boundary layer thickness is assumed be 0.1 mm. The dynamic shape factor is 1.0.

Multi component aerosol model

20 aerosol size classes are simulate. The lower boundary is $0.01 \times 10^{-6}$ m, the upper is $50 \times 10^{-6}$ m.
The MAG (see above) models the coupling between particle condensation and the aerosol model MAEROS.
The atmospheric conditions calculated in the thermal hydraulic part are boundary conditions of the aerosol part. The contribution of condensation and evaporation on/from hygroscopic aerosol particles to water and steam mass and energy balances are not simulated in these calculations.

List of aerosol deposition areas

The numbers given in the specification are used:
Table 5.4: Aerosol deposition areas

<table>
<thead>
<tr>
<th>Area</th>
<th>Area (m²)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Floor</td>
<td>7 m²</td>
</tr>
<tr>
<td>Ceiling</td>
<td>7 m²</td>
</tr>
<tr>
<td>Side wall</td>
<td>17 m²</td>
</tr>
</tbody>
</table>

Input data that differ from the specification:

The area of the artificial wall part no. 10 simulating the heat loss through the structures attached on the outside of the vessel is smaller than proposed, see table 5.5:

Table 5.5: Aerosol deposition area of wall part No. 10

<table>
<thead>
<tr>
<th>Component</th>
<th>Area (m²)</th>
</tr>
</thead>
<tbody>
<tr>
<td>K123</td>
<td>1.55</td>
</tr>
<tr>
<td>K148</td>
<td>1.9</td>
</tr>
<tr>
<td>K188</td>
<td>1.25</td>
</tr>
<tr>
<td>K186</td>
<td>1.25</td>
</tr>
</tbody>
</table>

In the calculations for K123, K186 and K188 all particles consist of the injected aerosol component and water. The water phase dominates. Since MAEROS uses for all aerosol components only one constant density, a value of 1100 m³/kg (close to water) was input. In the calculation for K148 most of the silver particles are dry. Since they determine the silver concentration, a density of 8000 m³/kg (somewhat lower than the theoretical one) was input. For K148 aerosol injection rate was reduced to half of the proposed value, in order to get close to the first aerosol concentration after the end of injection.
NRI

Experimental device description

- Control volume

It was decided to describe the experiment by a single control volume. It is expected that the impossibility to model local effects like different temperatures near walls is by far counterbalanced by avoiding artificial stratification effects of the code that can treat only pressure and inertia driven flows between volumes. It also seems that the experimental volume was well mixed.

The total inside volume was taken from the specification as 10.595 m. To follow its cylindrical shape (except for the doorways) it was replaced by a stepwise rectangular shape.

This is especially important in the lower part of the vessel to properly calculate the sump height, surface and its contact with walls. The division also copies that one proposed in the specification for walls.

A virtual control volume representing the environment with atmosphere temperature 20 °C was added as a time constant volume, this means that the thermodynamics is not calculated be MELCOR and the parameters are fixed. Mass and heat input to this volume are conserved, however.

- Heat structures

The external heat structures as proposed in specification table 1 were used. Though MELCOR can model cylindrical structures, it cannot model sectors of them. Only a half of a cylinder or a full cylinder is allowed. There was a choice either to reorganize the structures completely or to keep them as proposed but replace them by flat (rectangular) ones. The second option has been selected. The inner surface area from table 1 in the specification was conserved, this means that the total volumes of structures, their thermal capacities and their outer surfaces will be smaller than in reality.
To compensate for this and because the thermal hydraulic calculation indicated tendencies to higher heat-up of the volume than given in some important time points, the virtual wall area recommended has been increased to 5 m\(^2\) while keeping its thickness, besides 2 m\(^2\) of similar but horizontal virtual wall was added at the bottom of the sump. The reason for this was the observation of conditions much closer to equilibrium between the atmosphere and the sump in the calculation comparing to experimental results. As MELCOR is known to treat very exactly such conditions, possible explanation could be that the stand of the experiment contributed strongly to heat removal from the volume. For both virtual walls, the water film and water condensation were allowed (though this is unimportant for the second one constantly submerged in the sump). On the other hand, aerosol sedimentation on these structures was forbidden to avoid artificial increasing of the deposition area.

Because the contact with changing sump inside the vessel is important, the structure 4 in table 1 of the specification was divided into 4 structures 41, 42, 43, 44. The first of them is horizontal, at the lowest vessel position, the others are copying the circular shape of the vessel as secants.

MELCOR automatically treats heat structures as deposition areas for aerosols. It is possible to disable this function or change orientation of any of these structures, but not to change their area. This was used to disable aerosol deposition on virtual walls as noted above. Some disagreement occurred between the data for vertical walls, ceilings and floors in the specification and those declared in MELCOR. The area of vertical walls in MELCOR is larger and that of ceiling smaller than recommended, but their sum differs by only 3.3 % (larger in MELCOR input). This discrepancy is considered acceptable. The difference in floor area was compensated for by adding a horizontal internal steel heat structure to MELCOR with the area 1.717 m\(^2\) and thickness 2 mm. It is representing mainly the internal equipment due to which the difference between external walls and the value recommended probably occurred. The overview of aerosol deposition structures is given in table 1 of the specification.

For all structures, the standard model of steam condensation on surfaces was enabled (default). This model assumes maximum film thickness 0.5 mm and adds the extra condensate to the sump. The new film flow tracking model was not used.

For all structures (except the virtual one submerged in the sump), the simple heat radiation GREY-GAS model was activated on both the internal and the external surfaces using the emissivity 0.9 for painted and 0.25 for zinc plated sheets.
Heaters used in some external structures in phase I was modeled by internal heat sources in the steady state tuning phase. These internal heat sources were used directly in the 1 cm thick innermost node of the insulation.

**Table 5.6:** Overview of aerosol deposition surfaces

<table>
<thead>
<tr>
<th>No</th>
<th>thickness steel [m]</th>
<th>thickness insulation [m]</th>
<th>type</th>
<th>heat transfer area [m²]</th>
<th>deposition area [m²]</th>
<th>settling area [m²]</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>0.025</td>
<td>0.075</td>
<td>ceiling</td>
<td>4.07</td>
<td>4.07</td>
<td>0</td>
</tr>
<tr>
<td>20</td>
<td>0.025</td>
<td>0.1</td>
<td>ceiling</td>
<td>0.235</td>
<td>0.235</td>
<td>0</td>
</tr>
<tr>
<td>30</td>
<td>0.037</td>
<td>0</td>
<td>ceiling</td>
<td>1.372</td>
<td>1.372</td>
<td>0</td>
</tr>
<tr>
<td>41</td>
<td>0.025</td>
<td>0.075</td>
<td>floor</td>
<td>0.717</td>
<td>0.717</td>
<td>0.717</td>
</tr>
<tr>
<td>42</td>
<td>0.025</td>
<td>0.075</td>
<td>slanted floor</td>
<td>0.892</td>
<td>0.892</td>
<td>0.870</td>
</tr>
<tr>
<td>43</td>
<td>0.025</td>
<td>0.075</td>
<td>slanted floor</td>
<td>0.617</td>
<td>0.617</td>
<td>0.575</td>
</tr>
<tr>
<td>44</td>
<td>0.025</td>
<td>0.075</td>
<td>slanted floor</td>
<td>1.843</td>
<td>1.843</td>
<td>1.513</td>
</tr>
<tr>
<td>45</td>
<td>0.002</td>
<td>0</td>
<td>internal floor</td>
<td>0</td>
<td>1.717</td>
<td>1.717</td>
</tr>
<tr>
<td>50</td>
<td>0.025</td>
<td>0.1</td>
<td>floor</td>
<td>0.235</td>
<td>0.235</td>
<td>0.235</td>
</tr>
<tr>
<td>60</td>
<td>0.037</td>
<td>0</td>
<td>floor</td>
<td>1.372</td>
<td>1.372</td>
<td>1.372</td>
</tr>
<tr>
<td>70</td>
<td>0.025</td>
<td>0.075</td>
<td>side wall</td>
<td>11.73</td>
<td>11.73</td>
<td>0</td>
</tr>
<tr>
<td>80</td>
<td>0.025</td>
<td>0.25</td>
<td>side wall</td>
<td>4.685</td>
<td>4.685</td>
<td>0</td>
</tr>
<tr>
<td>90</td>
<td>0.037</td>
<td>0</td>
<td>side wall</td>
<td>1.85</td>
<td>1.85</td>
<td>0</td>
</tr>
<tr>
<td>100</td>
<td>0.024</td>
<td>0</td>
<td>virtual, side</td>
<td>5</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>110</td>
<td>0.024</td>
<td>0</td>
<td>virtual, floor</td>
<td>2</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>total</td>
<td></td>
<td></td>
<td></td>
<td>36.619</td>
<td>31.336</td>
<td>7.000</td>
</tr>
</tbody>
</table>

- **Modeling the leak**

The leak was modeled by a flow path between the vessel internal volume and the environment with parameters as recommended. The length of the flow path is very small giving a very small friction resistance while the local resistance was used as recommended. This flow path has been closed by valve during the structures steady state stabilization period.
- **Initial conditions**

- **Thermal hydraulic conditions**

Calculation of the phase I was skipped. It would be rather complicated and the final conditions may differ from those given on the ISP44 CD. A small discrepancy was found in the initial conditions input. For the given temperature 109 °C and humidity 93 %, the steam partial pressure alone is higher that the given total pressure 1.05 bar. To compensate for this, the given humidity was ignored and the nitrogen and steam partial pressures calculated to match the total pressure. The given nitrogen mass was preserved. This leads to 75 % humidity. First calculations showed that the non-equilibrium between the sump and the atmosphere is hardly explainable even with the virtual heat structure, it disappeared in few minutes after the start of calculation. To slightly compensate for this, the total pressure was slightly increased and the atmosphere temperature slightly decreased within the measurement error band. This also leads to slightly closer agreement in the humidity. The initial conditions used in the input or calculated by MELCOR are:

**Table 5.7:** Definition of the initial phase II state in MELCOR

<table>
<thead>
<tr>
<th>parameter</th>
<th>value</th>
<th>treated by MELCOR as</th>
</tr>
</thead>
<tbody>
<tr>
<td>time</td>
<td>0 s</td>
<td>input</td>
</tr>
<tr>
<td>total pressure</td>
<td>1.06 bar</td>
<td>input</td>
</tr>
<tr>
<td>atmosphere temperature</td>
<td>108 °C</td>
<td>input</td>
</tr>
<tr>
<td>relative humidity</td>
<td>78.5 %</td>
<td>calculated</td>
</tr>
<tr>
<td>$N_2$ mole fraction in dry atmosphere</td>
<td>1.0</td>
<td>input</td>
</tr>
<tr>
<td>nitrogen mass</td>
<td>0.092998 kg</td>
<td>calculated</td>
</tr>
<tr>
<td>steam partial pressure</td>
<td>1.050067 bar</td>
<td>input**</td>
</tr>
<tr>
<td>sump temperature</td>
<td>100 °C</td>
<td>input</td>
</tr>
<tr>
<td>sump mass</td>
<td>2.11 kg</td>
<td>input</td>
</tr>
</tbody>
</table>

** calculated by hand as difference between the total pressure and $N_2$ partial pressure calculated from the equation of state

34
- Wall temperature profile

Tuning of the heat profile in the heat structures was a more difficult task. MELCOR has a steady state profile initialization option, but this proved first to be unstable for the given structures and failed most probably due to condensation on them. This conclusion is based on the fact that the failure was avoided for one best insulted wall 80 where condensation did not occur. The problem was corrected by changing a sensitivity coefficient, but the calculated profile was not quite stable in time and did not include the heaters power. For this reason, the profile was stabilized calculating 1 hour period between time -3600.0 s and 0.0 s during which also the inner vessel volume was kept at constant parameters and the wall heating mats were switched on between -3600.0 to -1020.0 s at 2500 W. Note that the aim was to obtain a reasonable approximation of the wall temperature profile using very rough approximation of the last hour of phase I, not a closer evaluation of parameters during the end of this phase that changed in reality. The time 1 hour was selected based on observing the changes in the wall temperature profiles.

- Sources of gas
  
  - Injection of steam

The injection of steam was modeled by a source of mass and a source of energy using the data from the specification. Because a slight rise in temperature and pressure was observed in the results which was not indicated a sensitivity study was performed where the source of energy has been replaced by enthalpy calculated by the code from mass and steam temperature recommended. The results were exactly the same as those where the source of steam energy was used.

- Sources of nitrogen

Two sources of nitrogen, the clearing and the carrier gas were modeled by a nitrogen mass source and temperature table taken from the specification, from which the code calculated the source of enthalpy.

The third nitrogen source is negative, it represents the sampling. It was modeled by a negative mass source and a negative energy source calculated by the code by multiplying the mass source by nitrogen specific enthalpy (extracted from the code by a control function).
- **Aerosol input**

- **General input to the RN package**

Only rare MELCOR input was needed and most parameters have been included as defaults.

Because the MELGEN code did not find any DCH package cards it printed out a very strong warning that there is no decay heat in the calculation, this was ignored. To facilitate a future transfer to a reactor case and to save effort in preparing input data, all default 16 material classes were used with the default numeration, i.e. CsOH was class 2, Ag class 12, water class 14, and CsI class 16 (automatic creation of this class is new in MELCOR 1.8.5). The other 12 classes were not used and the aerosol and vapor masses in them remained zero. The SC7120 was used to redefine the molecular mass of the 12 class from that of Sn to Ag, which is 107.87 kg/kmol. The other two aerosols, CsOH and CsI are representatives of their classes and so their molecular masses are correct.

A very important trick is to use the RNAGXXX card to define initial masses of aerosol in the atmosphere. They were defined 1E-10 kg for all three mass classes and all size sections. With exactly zero dry aerosol masses the whole package becomes inactive until first aerosols arrive and the water fog is stored and added to the first aerosols balance. Though it seems not influence aerosol dynamics very much, the results look ugly with no water aerosols before the first source and a water peak after.

Finally, to reduce printouts and calculation time, all vessel structures facing the environment were excluded from deposition areas. More important, the left surfaces of virtual heat conducting structures facing the vessel interior were also excluded.

- **Hygroscopic model**

Originally, the hygroscopic model was activated by setting: RN1002 1

It resulted in very fast depletion of airborne aerosols which was much higher than anything observed in KAEVER experiment. The conclusion is that either a severe error in the input data exists or the hygroscopic model has some deficiencies yet. We are planning turn to code developer with this question. For the reference calculation, the present code default which is not
to use this model, was applied. As a sensitivity study, the hygroscopic model has been used, the aerosols depletion results are included in this report.

- **Aerosol parameters**

The 1.8.5 version defaults were used for size sections, 10 sections with the smallest particle diameter 0.1 µm and the largest one 50 µm. The particle density was kept at 1000 kg/m³ which is the code default. It is a problem that this parameter cannot be changed in time or at least input for individual components. The dry aerosol density averaged over total mass was calculated as 4375.7 kg/m³, the input density is more appropriate to fog, which indeed represents most aerosols during the calculation. In the most important period of aerosol depletion after stopping their source, the particle density was about 1500 kg/m³. As a sensitivity calculation, the particle density was set to 1500 kg/m³ with the hygroscopic model remaining switched off. Though this may represent better the real aerosol behaviour, because of small difference to the original results, the results with 1000 kg/m³ aerosol density were used as reference.

Three components were used in agreement with the code defaults, component 1 for all non-hygroscopic aerosols, component 2 for water and component 3 for hygroscopic groups CsOH, CsI. Gas groups noble gases (with zero masses in this problem) and I were also added to component 3. This input enables switching on the hygroscopic modeling while the extra component should have no effects if this modeling is off.

In agreement with the recommendations, the dynamic shape factor and agglomeration shape factor have been set to 1.0 (which are also defaults). Other special particle properties were also left as default. The coefficients in aerosol transport equations, dependent on pressure and temperature were requested to be calculated inside the code instead of their input.

- **Aerosol sources**

The three aerosol sources have been defined using RNASXXX cards selecting tabular functions defining their intensity versus time. On these cards, the log-normal distribution can be selected and its parameters input. The mass median diameter 0.518 µm (equal to volume median diameter) and standard deviation 1.3 were input. The other option would be to use geometric mean diameter. There seems to be some disagreement among the geometric median, volume median and standard deviation as recommended. An agreement could be reached if the
geometric median would be a geometric mean and the standard deviation would be higher, about 1.45.

GRS/IPSN

"Open" calculation

Input Different from Specifications

The wall number 10 used as an artificial wall to regulate heat transfer out of the containment in order to optimize the given thermal-hydraulic condition has its surface set according table 5.8:

<table>
<thead>
<tr>
<th>Case</th>
<th>Surface (m²)</th>
</tr>
</thead>
<tbody>
<tr>
<td>K123</td>
<td>3.65</td>
</tr>
<tr>
<td>K186</td>
<td>2.50</td>
</tr>
</tbody>
</table>

An additional layer of steel of thickness 0.002m has been added as a coating surface on each insulated wall.

The initial and transient thermal hydraulic conditions for phase I are different from those suggested in the CD-Rom. They are actually closed to those communicated later on in December 2000.

Short Description of Analytical Models

We give in the following section the main characteristics used for applying the aerosol module of ASTEC-CPA. We focus essentially on the aerosol properties, the key-point of the ISP44 being the simulation of aerosol behavior.
**Thermal hydraulic module description**

The thermal hydraulic model deals with the interaction of a homogeneous mixture of steam and non-condensable gases in contact with several walls (10) and a sump modeled by a water free surface and walls.

It is able to evaluate pressure and temperature build-up and history, local temperature and pressure distributions, energy and local heat transfer to heat conducting structures, local gas distributions (both steam and incondensable gases), hydrogen distribution, water distributions, mass and volume flows for the release of fluids through openings and leakages.

Calculations are being performed for single gas compartment containment.

One of the key assumptions made in the CPA code is the well-mixed atmosphere hypothesis by volume only.

The simulation of heat and mass transfer between a zone and the atmosphere is made using free and forced convection models, a radiation model, and the Stefan condensation and evaporation model when the thermal status of the zone requires its application.

Heat conduction in walls is described by the Fourier 1D equation.

Walls and other internal structures are described by using a plane geometry.

Such walls can consist of several layers of different materials possibly separated by air-filled gaps. We use steel and insulation as prescribed in the ISP44 Report.

Each material can be subdivided into an arbitrary number (10) of layers with different thicknesses for solving the heat conduction equation provided they are defined by giving their heat conductivity, specific heat, and density values (see ISP44 Report).

**Aerosol Module Description**

Number of Class Sizes 20
Number of Chemical Aerosol Components (Water + Aerosol)

K123 - 2
K186 - 3

Lowest & Highest Particle Diameter Limits
1.D-08 & 1.D-04

Relative Accuracy Criterion for Aerosol Transport
0.20

Relative Accuracy Criterion for Aerosol Agglomeration
0.20

Use of an Explicit Integration

Maximum Time Step
20 s

**Agglomeration Model**

Use of Collision Efficiency: Pruppacher & Klett Model

Particle Slip Coefficient
1.37

Particle Sticking Probability
1.0

Use of Aerosol Contribution to Gas Density

Molecular Weight of Gas:
23.

**Thermophoresis Model**

Thermal Accomodation Factor
1.

Ratio of Gas to Particle Heat Conductivities
0.037

**Diffusiophoresis Model: Waldmann & Schmitt**

Diffusion Boundary Layer Thickness (m)
0.001

Use of Condensation Model on Aerosols

DYNAMC = 0: Kohler equation, DYNAMC = 1: Mason equation

Use of Solubility Feedback of Hygroscopic Aerosols on Thermal Hydraulics

Kelvin Effect (N/M) – Surface Tension Value
K123 – Surten = 0
K186 – Surten = 0

No Aerosol Nucleii Added for Condensation

Number of Time Steps for Condensation Growth Calculation
5

**Brownian Agglomeration**

Agglomeration Shape Factor (GAMMA)
1.0

Dynamic Form Factor (CHI)
1.0

Rate of Dissipation of Turbulent Energy
0.001

Sedimentation: Densities (kg/m³)
K123 – Density = 1100
K186 – Density = 1100
"Blind" calculation

- **Code version**

The calculations for ISP44 were performed with ASTEC version 0.3 from October 2000. No modifications were introduced into this version. Module CPA was activated only in the calculations.

- **Nodalization**

The test containment was modeled by one non-equilibrium zone with a volume of 10.595 m$^3$. The sump surface, i.e. the interface area between the liquid and the gaseous zone part was 3 m$^2$. The effect of the cylindrical vessel that the sump surface varied with the sump water level could not be modeled. The environment surrounding the test containment was modeled by one equilibrium zone.

Both zones were connected by an atmospheric junction simulating small mass losses through the leaky door opening mechanism (Table 5.9). Cross section and pressure loss coefficient of the junction have been chosen according to the values proposed in the specification report$^6$.

<table>
<thead>
<tr>
<th>test</th>
<th>cross section [mm$^2$]</th>
<th>pressure loss coefficient [m$^{-4}$]</th>
</tr>
</thead>
<tbody>
<tr>
<td>K148</td>
<td>26</td>
<td>27000</td>
</tr>
<tr>
<td>K187</td>
<td>47</td>
<td>27000</td>
</tr>
<tr>
<td>K188</td>
<td>102</td>
<td>27000</td>
</tr>
</tbody>
</table>

The components water, steam and air were modeled in the zones. Component air was defined with the properties of nitrogen and simulated the nitrogen in the test. The aerosol module of CPA

$^6$ The proposed values in the specification report were increased by a factor of 100 for the cross section and by a factor of 10000 for the pressure loss coefficient. Thus, the resulting mass flow through the junction was the same as if the original values would have been issued.
requires the definition of either component air or a mixture of the components nitrogen and oxygen. The oxygen in the vessel was removed in the tests already during the initial flushing of the vessel with steam in the preparatory phase.

The walls of the test vessel have been modeled by nine plate type structures. The meshing of the material layers of the structures was equidistant. The steel layer has been subdivided into 2 layers, an inner layer of 2 mm with 2 meshes in contact with the containment atmosphere and a second layer with 5 meshes for the remaining thickness. This subdivision became necessary because in the calculation of the condensation heat transfer the temperature of the first mesh was used instead of the surface temperature, thus avoiding the iteration of the surface temperature. Therefore, it is advised to use thin meshes for the material layer in contact with the atmosphere when using that option.

The insulated wall parts were covered by a thermal insulation layer (10 meshes) and an additional steel layer (2 meshes) of 2 mm thickness.

As proposed in the specification report the cooling fin effect of the door opening mechanism was modeled by an artificial structure (structure 10) in contact with the vessel atmosphere. The surface of this structure was adjusted such that the calculated and the measured atmosphere temperature were in good agreement in all of the three calculated tests.

An additional structure (structure 11) was modeled to simulate the room walls surrounding the test facility. This structure was in contact with the environment zone by convective heat transfer and with the outer surfaces of the vessel wail structures by radiative heat transfer.

The heat transfer modes on the internal side of the structures in contact with the vessel atmosphere were free and forced convection, condensation and wall-gas-radiation. The structures with orientation type 'floor' (structures 4, 5 and 6) were in contact with zone part sump of the non-equilibrium zone. The heat transfer modes were limited here to free and forced convection. The heat transfer modes on the outer side of the structures in contact with the environment zone were free and forced convection, condensation and radiation from wall to wall.

\[ \text{Option SMTP ‘FIRST\_LAYER\_TEMPERATURE’ in the input data} \]
The thermal properties of the structure materials were set as proposed in the specification report.

- **Aerosol model parameters**

The aerosol deposition areas in the vessel were set according to the specifications, i.e. 7 m\(^2\) for floor and ceiling and 17.6 m\(^2\) for the side walls.

**Table 5.10:** Main characteristics of vessel wall structures

<table>
<thead>
<tr>
<th>structure</th>
<th>area [m(^2)]</th>
<th>orientation</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>4.07</td>
<td>ceiling</td>
</tr>
<tr>
<td>2</td>
<td>0.235</td>
<td>ceiling</td>
</tr>
<tr>
<td>3</td>
<td>1.372</td>
<td>ceiling</td>
</tr>
<tr>
<td>4</td>
<td>4.07</td>
<td>floor</td>
</tr>
<tr>
<td>5</td>
<td>0.235</td>
<td>floor</td>
</tr>
<tr>
<td>6</td>
<td>1.372</td>
<td>floor</td>
</tr>
<tr>
<td>7</td>
<td>11.73</td>
<td>side wall</td>
</tr>
<tr>
<td>8</td>
<td>4.685</td>
<td>side wall</td>
</tr>
<tr>
<td>9</td>
<td>1.85</td>
<td>side wall</td>
</tr>
<tr>
<td>10</td>
<td>2.35</td>
<td>side wall</td>
</tr>
<tr>
<td>11</td>
<td>1000</td>
<td>side wall</td>
</tr>
</tbody>
</table>

**Table 5.11:** Thermal properties of structure materials

<table>
<thead>
<tr>
<th>material</th>
<th>conductivity [W/m/K]</th>
<th>heat capacity [J/kg/K]</th>
<th>density [kg/m(^3)]</th>
</tr>
</thead>
<tbody>
<tr>
<td>steel</td>
<td>45</td>
<td>480</td>
<td>7850</td>
</tr>
<tr>
<td>insulation</td>
<td>0.091</td>
<td>840</td>
<td>110</td>
</tr>
</tbody>
</table>

The injected aerosols were simulated by one component, respectively three components in tests K 187, and the water condensing on the aerosols by an additional component. The components were assumed to be homogeneously mixed. They were divided into 20 size classes between 0.01 μm and 100 μm.
The density of the aerosols was assumed to be 1100 kg/m$^3$ for tests K 187 and K 188 where the water condensed on the aerosols dominated the average particle density. In test K 148 (silver aerosol), the Kelvin effect hindered condensation on small particles. Therefore, the mean density of the aerosols was assumed to be 5000 kg/m$^3$, which is approximately 50 % of the theoretical density of silver.

The solubility (Van't Hoff factor) was set according to the specifications to 2 for component CsOH, to 1.7 for component CsI and to 0 for component Ag. The feedback of the hygroscopicity of the aerosols on the thermal hydraulic in the vessel was taken into account. Dynamic form factor and agglomeration form factor were set to 1.

The Kelvin effect was taken into account in the calculation of test K 148 with the insoluble silver aerosols. In the three-component test K 187 it was assumed that the silver particles are well mixed with the other components because of the simultaneous injection of the three components and the comparable size distribution. The Kelvin effect could be neglected in tests K 187 and K 188 because of the high solubility of the particles.

- Initial and boundary conditions

The initial and boundary conditions for the preparatory phase (phase 1) of the tests were set in the calculations different to the conditions specified on CD-ROM. Those conditions had been used in previous analyses with the code FIPLOC and were not the measured boundary conditions.

A transient of 100000 s was assumed for phase 1. The initial conditions were a pressure of 1.9 bar, a temperature of 104 °C and a humidity of 100 % for the non-equilibrium zone modeling the vessel, and a pressure of 1 bar, a temperature of 20 °C and a humidity of 80 % for the equilibrium zone modeling the environment.

The boundary conditions during phase 1 were as follows:

- Slightly superheated steam was injected at a rate of initially 7 g/s and later on 3g/s.
- Structures 1, 4 and 7 were heated with a total power between 2.4 and 2.5 kW in tests K187 and K188. Heat was distributed to the structures according to their surface ratio. The heating was turned off in test K148
- The air was withdrawn from the vessel by a negative nitrogen source at the beginning of phase 1.
- The condensed water in the vessel was withdrawn from the sump by a negative water source in tests K187 and K188 at the end of phase 1. The sump water was not withdrawn in test K148.

The boundary conditions specified on CD-ROM for phase 11 were used for the injection of steam and nitrogen carrier and clearing gas as well as for the removal of nitrogen due to probe taking. The heating of the walls was turned off in all three tests during phase 11. The aerosol injection rate was adjusted in all three tests in order to fit the calculated dry aerosol concentration to the first measured concentration after the end of aerosol injection into the vessel as it was suggested in the specifications.

**Table 5.12: Aerosol parameters**

<table>
<thead>
<tr>
<th>test</th>
<th>injected mass [g]</th>
<th>number median diameter [µm]</th>
<th>standard deviation</th>
<th>factor&lt;sup&gt;8&lt;/sup&gt;</th>
</tr>
</thead>
<tbody>
<tr>
<td>K148</td>
<td>4.3 (Ag)</td>
<td>0.516</td>
<td>1.4</td>
<td>0.5</td>
</tr>
<tr>
<td>K187</td>
<td>11.4</td>
<td>0.315</td>
<td>1.3</td>
<td>0.33</td>
</tr>
<tr>
<td></td>
<td>1.1 (Ag), 4.2 (CsOH), 6.1 (CsI)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>K188</td>
<td>16.7 (CsOH)</td>
<td>0.26</td>
<td>1.45</td>
<td>1.4</td>
</tr>
</tbody>
</table>

### 5.4 Comparison of Analytical and Experimental Results

According to the codes used the results of the 10 contributions are divided into 2 groups, i.e. the MELCOR group (JRC, KAER, NRI, STUD, VEIK) and the miscellaneous MISCEL group (GRS,

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<sup>8</sup> The injection rate given in the specifications was multiplied with this factor to obtain in the calculation the first measured dry aerosol concentration after the end of the aerosol injection.
GRSIPSN, IJS, JAERI, RUB), which uses the codes ASTEC, ART/REMOVAL, COCOSYS and CONTAIN. The results of the four open calculations and the blind calculation are described separately.

5.4.1 Open Calculations

Of the open calculations the most important plots have been selected to give an impression of the results and the capability of the codes to calculate the different experiments with known experimental results. General explanations for all tests will be given together with the blind results.

5.4.1.1 Containment Pressure

The containment pressure for the 4 open calculations (K123, K148, K186, K188) is given in Fig. 5.1a to 5.4b.

The pressure calculated by the MISCEL group agrees generally well with the measurement. In some calculations for the test K123 and K186 however deviations occur. The MELCOR group shows a fairly good agreement for the tests K123 and K186 but deviations for the remaining tests.

The deviations in pressure can be explained by the simulation of the atmospheric temperatures and N₂ masses. For example IJS calculates a 0.5 bar too high pressure at the end of test K123 which is a result of a more than 10 °C too high atmosphere temperature. The overprediction of the pressure of test K148 by GRS-IPSN by 0.3 bar is consistent with a too high temperature. The spread in pressures of +/- 0.4 bar shown by the MELCOR group at the end of test K188 is mainly caused by different N₂ masses resulting from different leak rates.

5.4.1.2 Atmospheric Temperature

The atmospheric temperature is plotted in Fig. 5.5a to 5.8b.

For the 1 component test K188 a good agreement between measurement and calculation has been achieved. For the other tests a more or less large deviation can be seen.
5.4.1.3 Relative Humidity and Volume Condensation Rate

The most important thermal hydraulic variables influencing the aerosol behaviour are the humidity and the volume condensation rate. The humidity determines the condensation on hygroscopic particles, the volume condensation rate determines the condensation on hygroscopic and insoluble particles. Since the error band of humidity measurement is very high (+- 10 %) it has to interpreted carefully. Often the signal rises to 110 % or more. In a technical system like the KAEVER test facility however only a maximum of 100 % is possible. Signals below 100 % indicate that the atmosphere might have been superheated. The volume condensation rate cannot be measured, only a comparison between the codes is possible.

The relative humidities and volume condensations rates are plotted in figures 5.9a to 5.16b. (Remark: In all plots the humidity shown for IJS is wrong due to a computational error. As reported by IJS on the comparison workshop the humidity was 99.9 % during the depletion phase.)

- K188

In test K188 the measurement signal for the relative humidity is generally about 110 % except for the aerosol injection phase, here it is below 100 %. This indicates that the atmosphere might have been superheated during the injection phase and saturated during the depletion phase with a humidity of 100 %. The codes generally give qualitatively similar results: A more or less stronger superheating during the injection phase or at least during a part of it and a humidity of 100 % in the depletion phase. The data given by JRC and STUD show a humidity of only 99 %. However the amount of airborne water calculated indicates saturation (see also discussion of test K148).

The volume condensation rate (i.e. steam condensation by equilibrium fog formation on the particles) cannot be measured. MELCOR does not provide this as an output variable. The data given by this group cannot be used for comparison.

In the MISCEL group RUB and GRS/IPSN calculate during the aerosol depletion phase volume condensation rates about $2 \times 10^{-5}$ kg/s m$^3$. GRS calculates $1.3 \times 10^{-5}$ kg/s m$^3$. The reason for the difference is caused by a different application of the heat transfer model. The IJS result reflects only hygroscopic condensation on the particles.
The measurement signal for the relative humidity is always above 110 % during the injection phase it increases even. This is in contrast to the test K188 and physically not explainable since almost the same test procedures were used. The code results are very similar to that of test K188.

Test K123 was the only one with wall heating during the aerosol phase. The humidity measurement signal is always near 90 %. Because of the large uncertainty of the measurement this is no prove that in the experiment the atmosphere was really superheated. But it indicates that the volume condensation rate was smaller than in the other test or even zero. This consistent to the volume condensation rates calculated by the MISCEL group which are much lower than those for the other tests: GRS-IPSN and RUB calculate $1.3 \times 10^{-5}$ kg/s m$^3$, GRS $0.8 \times 10^{-5}$ kg/s m$^3$. IJS shows only at the end of the aerosol injection and some minutes during the beginning of the depletion phase a small hygroscopic condensation on the particles. The calculated humidities are similar to those of the other tests. The two times when they decrease to a minimum during the injection phase are consistent to the measurement.

The measurement signal shows values above 115 % and cannot be used for comparison. In contrast to the other experiments the codes do not calculate a superheated atmosphere during the injection phase. During the depletion phase they calculate 100 % humidity, except for JRC and STUD which show 99 % as for the other test. These calculations however simulate a lot of airborne water even before the aerosol injection starts. This indicates a simulation of a saturated atmosphere.

### 5.4.1.4 Total Dry Aerosol Concentration

As described in [23] the aerosol injection rate was not measured but calculated. The measured aerosol concentration and composition for a single point in time was given to the participants as a starting point for the aerosol depletion part of their calculation. Since in many cases participants did not meet this starting point, in the evaluation of the results more importance is
given to the comparison of the experimental and calculated aerosol depletion rates than to the absolute values of the concentrations.

The total dry aerosol concentration is the concentration of the aerosol material without water. It is given in Fig. 5.17a to 5.20b for the tests K123, K148, K186 and K188. There are some deviations to the starting point at the beginning of the depletion phase. This is less important for the evaluation since the particle growth by agglomeration is small in all tests. With some exceptions the gradient of the dry aerosol concentration decrease is fairly well calculated. But several calculations have larger deficits in other aerosol results like the airborne water content and the particle size distribution.

**Test K148 with non hygroscopic aerosol material (Ag)**

In the MELCOR group KAERI and Studsvik results show good agreement, but KAERI results have almost no airborne water. The Studsvik results show too much airborne water, which does not agree with the calculated slow aerosol decay. In this calculation Ag was treated as soluble aerosol. The JRC and VEIKI results strongly overestimate the aerosol decay. They do not calculate particles <1\(\mu\text{m}\) and therefore the Kelvin effect cannot have any influence on the calculations. In the other MELCOR results there is no indication that the Kelvin effect is treated.

In the MISCEL group all calculated Ag concentrations, except RUB results, show good agreement with the experimental data, but the IJS and JAERI results have no airborne water. RUB underestimates the aerosol decay since it simulates no airborne water although it shows a volume condensation. The GRS and GRS-IPSN calculations with COCOSYS and ASTEC show a large amount of airborne water which is condensed on a fraction of large particles due to the Kelvin effect. The fraction of the small Ag particles stays dry and depletes slowly.

**Test K123, K188, K186 with hygroscopic aerosol materials (CsI, CsOH, Ag +CsOH)**

The results of both groups, with some exceptions in test K123, show good agreement with the experimental data. In test K123 the last two measurement points are not regarded in the evaluation, since they are not reliable. JRC strongly overestimates the aerosol decay, GRS, GRS-IPSN and RUB overestimate the decay of CsI (K123), IJS and JAERI underestimate the decay of CsI. In the IJS calculation the droplet growth by volume condensation is not considered. It simulates the droplet growth only by hygroscopicity at almost saturated conditions.
(see thermal hydraulic part). KAERI and VEIKI calculated no solubility effect because of problems with the solubility model in MELCOR.

The different aerosol material solubilities in the three tests cause differently fast depletions of the measured dry aerosol concentrations. The solubility and the order of depletion are given in Table 5.13 a and b. In the JRC, VEIKI, IJS and JAERI calculations the order of depletion in the tests deviates from the measured order for different reasons. NRI calculated only test K187.

**Table 5.13a:** Solubility and measured order of depletion

<table>
<thead>
<tr>
<th></th>
<th>Ag</th>
<th>CsI</th>
<th>CsOH</th>
</tr>
</thead>
<tbody>
<tr>
<td>Van't Hoff factor</td>
<td>0.</td>
<td>1.7</td>
<td>2.0</td>
</tr>
<tr>
<td>Order of depletion in tests</td>
<td>K 148 &lt; K 123 &lt; K 188</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Table 5.13b:** Calculated order of depletion

<table>
<thead>
<tr>
<th>Code</th>
<th>Participation</th>
<th>Comparison with measurement</th>
</tr>
</thead>
<tbody>
<tr>
<td>MELCOR</td>
<td>KAERI</td>
<td>Order OK, but almost no airborne water</td>
</tr>
<tr>
<td></td>
<td>Studsvik</td>
<td>Order OK but different aerosol parameters</td>
</tr>
<tr>
<td></td>
<td>JRC</td>
<td>Decay Ag &gt; decay CsI (discrepancy)</td>
</tr>
<tr>
<td></td>
<td>VEIKI</td>
<td></td>
</tr>
<tr>
<td></td>
<td>NRI</td>
<td>Only K 187 calculated</td>
</tr>
<tr>
<td>COCOSYS</td>
<td>GRS / RUB</td>
<td>OK</td>
</tr>
<tr>
<td>ASTEC</td>
<td>GRS / IPSN</td>
<td></td>
</tr>
<tr>
<td>CONTAIN</td>
<td>IJS</td>
<td>Decay Ag ≈ decay CsI (discrepancy)</td>
</tr>
<tr>
<td>ART/REMOVAL</td>
<td>JAERI</td>
<td>Decay CsI &gt; decay CsOH (discrepancy)</td>
</tr>
</tbody>
</table>
5.4.1.5 Total Wet Aerosol Concentration

The total wet aerosol concentration includes the total dry aerosol and the airborne water concentrations. It is given in Fig. 5.21a to 5.24b. With some few exceptions the codes can not calculate the measured data. Only for test K188 (and RUB for test K186) the MISCEL group can meet the data. But the photometer measurement of the total wet aerosol concentration is not very accurate. Especially the measured decay of the wet aerosol concentration is uncertain.

5.4.1.6 Droplet Mean Diameter

Fig. 5.35a to 5.38b show the droplet mean diameter. The photometer measured droplet size is not very accurate. An example is the unexplained behavior of the measured droplet size in K186. In all tests the measured sizes are definitely too small.

5.4.1.7 Aerosol Size Distribution

The aerosol size distribution for test K148 at the time t=1000 s after the end of the aerosol injections is given in Fig. 5.25 to 5.34. In contradiction to the measurement some results show an almost dry aerosol (RUB, KAERI, JAERI, IJS). GRS and GRS-IPSN calculated a bi-modal size distribution caused by the Kelvin-effect, which is the reason for the slow decay even at high airborne water concentrations. There is no indication that the Kelvin-effect is treated by the other participants. In the JRC and VEIKI calculations no particles < 1µm are considered. In the Studsvik calculation the aerosol mass is distributed on three size classes only. It shows much water, this is in contradiction to the rather slow decay of the dry aerosol.

5.4.2 Blind Calculation (K187)

5.4.2.1 Thermal-hydraulic variables

The containment pressure and the temperatures of the atmosphere, the sump and the walls of test K187 were given for three points in time to the participants prior to their calculations: At the start of phase 2 (0 h) and at the begin and the end of the aerosol injection (13.33 and 15.33h)
• Containment Pressure

Fig 5.39 gives the pressure histories of test K187. All participants of the MISCEL group calculate the pressure fairly accurate, both the pressure increase during aerosol injection and the decrease during the aerosol depletion phase. The MELCOR group shows a spread of ± 0.2 bar (approximately 10 per cent). This is caused by different leak rates resulting in different nitrogen masses in the containment. The pressure calculated by NRI is influenced in addition by an overprediction of the atmospheric temperature.

• Atmospheric Temperature

The atmospheric temperatures are given in Fig. 5.40. The temperature decreases by 10 K from 0 to 5 h, then it increases slightly during the aerosol injection and decreases again during the depletion phase.

The predictions of the MISCEL group are quite well. The spread in the MELCOR group is a little bit larger. Only the results for NRI have a very large deviation and do not meet the general qualitative behavior.

• Relative Humidity

The humidity measurement (Fig. 5.52a and 5.52b) shows values above 110 %. It cannot be used for comparison. As in the open tests K188 and K186 the codes calculate generally humidities below 100 % during the aerosol injection phase and at 100 % during the depletion phase. Exceptions are STUD and JRC which show values about 99 %. This does not agree with the large amount of calculated airborne water. (Remark the plot for IJS wrong – according to IJS the real value is 99.9 %).

• Volume Condensation Rate

As in the open calculations the data given by the MELCOR calculation do not represent the volume condensation (Fig. 5.53a and 5.53b).

In the MISCEL group RUB and GRS-IPSN calculate during the aerosol depletion phase volume condensation rates above $2 \times 10^{-5} \text{ kg/s m}^3$. GRS below this value. The reason for the difference is caused by a different application of the heat transfer model. The IJS result reflects only the
hygroscopic condensation on the particles. The stand alone code REMOVAL used by JAERI does not calculate a volume condensation.

5.4.2.2 Aerosol Variables

- Dry Aerosol Concentration

Fig 5.54a and 5.54b show the total dry aerosol concentration for the depletion phase. After the aerosol injection the measured data decrease with an approximately linear gradient in the logarithmic presentation.

The calculated data give the tendency of the experimental behavior quite well, but the scatter of the data is about one order of magnitude (with two exceptions which have a larger scatter). Three calculations predict the correct initial concentration of the depletion phase. To overcome the shortcomings in the MELCOR solubility model some deviations from the experimental conditions are used in the MELCOR applications. In the KAERI, VEIKI and NRI calculations the solubility effect is not calculated. In the Studsvik calculation some aerosol parameters (e.g. shape factors) are modified incorrectly.

In the MISCEL group the GRS, RUB, GRS-IPSN and JAERI calculations agree well with the measurement. The initial concentration of RUB is too high. In all JAERI calculations volume condensation is not treated. The concentrations in the IJS calculations are too high resulting from a too high initial concentration but the gradient of the aerosol depletion is correct. In the IJS calculation volume condensation is not regarded. The GRS-IPSN calculation overestimates the aerosol depletion somewhat. The GRS-IPSN and RUB volume condensation rates are higher than the GRS one.

Fig 5.57 to 5.59 give the calculated concentrations of Ag, CsI and CsOH and the measured concentrations at two points of times. Although there is a characteristic difference in the aerosol behavior of the 3 species (hygroscopicity, material density, etc.) all 3 plots show the same depletion behavior and do not differ from the total aerosol behavior measured. The composition of the three components is almost the same in all particles at the two measurement times (Table 5.14). The aerosol generation procedure applied promoted the good mixing of the components.
### Table 5.14: Component mass fraction in K187

<table>
<thead>
<tr>
<th>Measurement time [h]</th>
<th>K187 mass fraction [%]</th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Ag</td>
<td>CsI</td>
<td>CsOH</td>
</tr>
<tr>
<td>7.2</td>
<td>13.2</td>
<td>54</td>
<td>32.8</td>
</tr>
<tr>
<td>7.7</td>
<td>14</td>
<td>48</td>
<td>38</td>
</tr>
</tbody>
</table>

- **Total Wet Aerosol Concentration**

The total wet aerosol concentration is given in Fig. 5.55a and 5.55b for the time period from 6 h to 11 h.

The experimental data increase during the injection phase up to 15 g/m$^3$ and then steadily decrease to 0.3 g/m$^3$ at 9.5 h where they level out. Again the photometer measurement is not very accurate. Especially the measured decay of the wet aerosol concentration by almost two orders of magnitude is not certain for the reasons already mentioned.

Only one calculated concentration matches the experimental data quite well, both the tendency and the actual values (IJS). But in this calculation volume condensation is not considered and the airborne water results only from the solubility effect. In the other calculations the increase of the wet concentration is generally calculated qualitatively correctly but then the results remain at a constant value. Only the MELCOR calculation of KAERI decreases again, but to a too low value. KAERI does not calculate the solubility effect and thus the results indicate almost no airborne water until 8.5 h. VEIKI and JRC start already with high concentrations.

Studsvik, JRC, VEIKI, NRI, GRS, RUB and GRS/IPSN results show a good agreement with the maximum of the total wet concentration in the injection period but have no or different decays of airborne water in the aerosol depletion period. JAERI has submitted no data.
• Droplet Mean Diameter

Fig. 5.56a and 5.56b give the comparison of the droplet mean diameter. The experimental data show a nearly constant value between 1 and 2 µm. This size is definitely too small as mentioned above.

During the aerosol depletion phase most calculated data show a nearly constant behavior. The GRS, GRS-IPSN and RUB calculations indicate a mean droplet size of approximately 7 µm in the depletion phase. In the IJS calculation without volume condensation the mean droplet size is 2-3 µm. All of the MELCOR-group except Studsvik and JRC carried out calculations without regarding the solubility effect. The resulting droplet sizes are 1.5 - 3.5 µm. In the Studsvik calculation the droplet size is about 4 µm for t < 8.2 h.

• Aerosol Size Distribution

The aerosol size distribution for test K187 at the time t=1000 s after the end of the aerosol injections is given in Fig. 5.60 to 5.70. The measured droplet size distribution (Fig. 5.60) refers to the calculated wet aerosol size distribution. For particle diameters > 10 µm the measured sectional aerosol concentrations seem to be too high for the large droplets. Only the JAERI result shows no water on the aerosol. In all other calculations except NRI the airborne water is equally distributed on the aerosol particles, i.e. the ratio of the water mass to the aerosol material mass is equal for all particle size classes. In the NRI calculation particles < 1 µm carry relatively more water than larger particles. In the VEIKI and JRC calculations the distributions are cut at 1 µm because smaller particles were ignored in these calculations. The calculated KAERI aerosol size distribution shows much airborne water, which is in contradiction to the time-dependent variables dry and wet total aerosol concentrations (compare Fig. 5.54a and 5.55a).

5.4.3 Summary

Only in the stand alone aerosol codes ART/REMOVAL volume condensation and multi-component behavior was not treated. Table 5.15 and Table 5.16 summarize for the MELCOR and the MISCEL groups the main particularities of the calculations.
Table 5.15: Particularities of the MELCOR group calculations

<table>
<thead>
<tr>
<th>Participant</th>
<th>Code Version</th>
<th>Kelvin-effect calculated</th>
<th>Solubility effect calculated</th>
<th>Particularities</th>
</tr>
</thead>
<tbody>
<tr>
<td>KAERI</td>
<td>1.8.4</td>
<td>(no)*</td>
<td>(yes)</td>
<td>Code changed for separate treatment of soluble and insoluble aerosol components; solubility effect unefficient, no volume condensation on particles</td>
</tr>
<tr>
<td>JRC</td>
<td>1.8.4</td>
<td>(no)*</td>
<td>yes</td>
<td>JRC and VEIK similar input but different code version, only particles &gt; 1 µm simulated</td>
</tr>
<tr>
<td>VEIK</td>
<td>1.8.3</td>
<td>no</td>
<td>no</td>
<td>JRC and VEIK similar input but different code version, only particles &gt; 1 µm simulated</td>
</tr>
<tr>
<td>STUD</td>
<td>1.8.4</td>
<td>(no)*</td>
<td>yes, also for Ag</td>
<td>Aerosol parameters changed: Dynamic shape factor from 1 to 2, diffusion boundary layer from $10^{-5}$ to $10^{-4}$ m, agglomeration shape factor differently from case to case</td>
</tr>
<tr>
<td>NRI</td>
<td>1.8.5</td>
<td>(no)*</td>
<td>no</td>
<td>Only K187 calculated</td>
</tr>
</tbody>
</table>

* no indications by analytical results that Kelvin effect is calculated

Table 5.16: Particularities of the MISCEL group calculations

<table>
<thead>
<tr>
<th>Participant</th>
<th>Code</th>
<th>Kelvin effect calculated in K148</th>
<th>Solubility effect calculated</th>
<th>Particularities</th>
</tr>
</thead>
<tbody>
<tr>
<td>GRS RUB</td>
<td>COCOSYS</td>
<td>yes (yes)</td>
<td>yes</td>
<td>The use of Kelvin effect in K148 leads to unreasonable results because of numerical problems with the condensation model of COCOSYS.</td>
</tr>
<tr>
<td>GRS-IPSN IJS</td>
<td>ASTEC</td>
<td>yes</td>
<td>yes</td>
<td>In all calculations no volume condensation</td>
</tr>
<tr>
<td>JAERI</td>
<td>ART/RENOVAL</td>
<td>no</td>
<td>yes (?)</td>
<td>In all calculations no volume condensation and no multi-component</td>
</tr>
</tbody>
</table>
6 Conclusions and Recommendations

The following observations and conclusions have been drawn by the participants and the ISP organizer.

The ISP44 comprises four open and one blind KAEVER aerosol depletion tests with three differently soluble aerosol materials and uniform thermal hydraulic conditions with slight volume condensation. These conditions are expected for longer periods in a LWR severe accident scenario.

All aerosol behaviour and thermal hydraulic processes essential for the KAEVER tests are modeled in the codes used. But some models are not applied because of model deficits and numerical stability problems. Only in the stand alone aerosol codes ART/REMOVAL volume condensation and multi-component behaviour are not treated.

Several discrepancies occurred concerning the tests with insoluble and slightly soluble aerosol materials. For the open test K148 with insoluble Ag-aerosol only two out of ten calculations are in good agreement with the measurement. For the open test K123 with slightly soluble CsI-aerosol no calculation has a satisfactory result. The discrepancies between the calculation and the measurement are mainly caused by an inaccurately calculated volume condensation rate, and an insufficient treatment of the Kelvin-effect and of the solubility effect. The thermal hydraulic boundary conditions for test K123 differed from those in the other tests and might not have been known exactly enough.

For the three tests with strongly hygroscopic CsOH (K186, K187 and K188) the quality of the analytical results of each participant is similar. In all MELCOR calculations, performed with three different code versions, the solubility effect is always poorly treated. Either the droplet growth and the aerosol depletion are significantly overestimated or the solubility effect is simply ignored.

The blind test K187 with a Ag-CsI-CsOH-aerosol mixture was well calculated by three out of ten participants using COCOSYS and ASTEC. The other calculations show larger deviations from
the experimental conditions (e.g. soluble materials treated as insoluble, volume condensation ignored) or incorrect results (e.g. no airborne water).

The three aerosol components were well distributed among all particles. The simple multi-component behavior in tests K186 and K187 is well calculated by all codes except ART/REMOVAL.

Uncertainties of initial and boundary conditions and of some measured parameters (e.g. aerosol injection rate) explain to a certain extent the spread of the consistent analytical results. The user influence on the aerosol results is high for the MELCOR-calculations of five participants. It is mainly caused by problems with the solubility model and the different attempts to overcome them. Without these attempts the droplet growth and the aerosol depletion was overestimated considerably.

Based on the general observations the following recommendations can be given.

The ISP44 with the fairly simple tests (single room geometry, steady state thermal hydraulic conditions) gives a good picture of both the capability of the codes and the users as well and of the quality of the experimental test facility. The agreement of the results with the measurements is not as good as expected. In particular the aerosol condensation modeling and the accuracy of related thermal hydraulic parameters should be improved.

- The solubility effect increases the growth of hygroscopic particles by condensation and enhances the aerosol depletion. An appropriate modeling is absolutely necessary. The solubility model in MELCOR needs some corrections.

- The Kelvin-effect may slow down the depletion of insoluble and slightly soluble aerosols in a condensing atmosphere. There are indications that the Kelvin-effect is not treated well by all codes except ASTEC and COCOSYS. The modeling of the Kelvin-effect should be checked. In some codes the numerical stability should be improved (e.g. COCOSYS).

For the calculations with a correct aerosol condensation treatment the largest discrepancies in the aerosol results is caused by the uncertain thermal-hydraulic variables "relative humidity" and "volume condensation rate". Appropriate guidance of the user is needed to define the thermal-hydraulic situation correctly (e.g. user manual, additional plot variables, user training). The multi-component behavior in the KAEVER tests was fairly easy to calculate, because the components
were well distributed among all particles. Experiments with partly mixed aerosol components are needed to validate the multi-component capability of codes.

ISP44 shows a large user influence on the results. Possible measures to reduce this influence are the improvement of code input assistance, user training, further benchmarks, etc.

The KAEVER experiments calculated for ISP44 had some measurement uncertainties (relative humidity, wet droplet size, aerosol injection rate, etc.). In future tests the measurement accuracy of important parameters should be improved.

At least a loose coupling of the stand alone-codes ART/REMOVAL with an appropriate thermal hydraulic model is recommended in order to simulate interaction phenomena and to avoid data transfer problems between the thermal hydraulic and the aerosol calculations.

In the ISP37 on test VANAM M3 all codes were already used except the new ones ASTEC and COCOSYS. The exercise comprised the depletion of a strongly hygroscopic aerosol in a multi-compartment geometry and was more complex than ISP44. Among the most uncertain variables and models analyzed were already "volume condensation rate", "relative humidity" and the solubility model. This demonstrates the necessity to perform several exercises on an important topic within a certain time.

Aerosol depletion in a condensing atmosphere is quite well understood and the models used are valuable tools for real plants, too. But the situation in real plants however is characterized by a much broader spectrum of conditions, and the complexity of the geometry, the thermal hydraulic transient and the aerosol generation has to be considered. In addition there are other important phenomena, e.g. dry and wet resuspension, the multi-component fission product behavior, aerosol removal by pool scrubbing and sprays, etc., which has to be taken into account in real plants.
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8 Appendix

Additional Contributions by the Participants

1. Jozef Stefan Institute (IJS), Ljubljana, Slovenia

2. Gesellschaft für Anlagen und Reaktorsicherheit mbH, Munich, Germany

3. Ruhr-University Bochum

4. Nuclear Research Institute plc., Rez, Czech Republic
1. Corrected calculations of relative humidity

The values of relative humidity in the report are wrong due to a programming error. The corrected calculations are presented on the following figures.

Test K123 Relative humidity in test vessel (correction of fig. 5.9a)
**Test K148** Relative humidity in test vessel (correction of fig. 5.10a)

**Test K186** Relative humidity in test vessel (correction of fig. 5.11a)
**Test K187** Relative humidity in test vessel (correction of fig. 5.52 a)

**Test K188** Relative humidity in test vessel (correction of fig. 5.12a)
2. IMPROVED SIMULATION OF TEST K123

For consistency, the same heat flux partitioning (inside steel: 70 %, outside insulation: 30 %) was used for all tests during which the test vessel was heated. As a result, a good agreement between measured and calculated thermal-hydraulic conditions was obtained for tests K188, K186 and K187. However, the agreement was not satisfactory for test K123, where the test vessel was heated during the entire experiment. The simulation of test K123 was thus repeated with a different heat flux partitioning, which was adjusted to obtain a good agreement between measured and calculated thermal-hydraulic conditions:

- during phase I (preconditioning phase):
  - inside steel: 70 %,
  - insulation: 30 %.
- during phase II:
  - inside steel: 20 %,
  - insulation: 80 %.

Representative results of the new simulation are presented in the following figures.

Test K123 Containment pressure (compare with fig.5.1a)
**Test K123** Atmospheric temperature (compare with fig. 5.5a)

**Test K123** Relative humidity (compare with first fig. in section 1)
Test K123 Total dry aerosol concentration (compare with fig. 5.17a)

Test K123 Total wet aerosol concentration (compare with fig. 5.21a)
3. CLARIFICATION ABOUT CONTAIN OPTION DROPOUT

In the simulations of all ISP-44 tests, the CONTAIN option DROPOUT was used. This option causes liquid from the atmosphere, which is formed due to condensation, to drop into a coolant pool at the cell floor. A thermal equilibrium between the coolant pool and the liquid coolant from the atmosphere is then established.

Thus, a consequence of the use of the option DROPOUT is that after the removal of the liquid from the atmosphere, the atmosphere is no longer saturated with vapor as soon as a small (infinitesimal) amount of vapor condenses.

In the ISP-44 calculations, the use of the option DROPOUT caused the atmosphere to become recurrently non-saturated due to vapor condensation on aerosols, as there was no more liquid coolant at saturation temperature present in the atmosphere. The atmosphere would periodically become saturated again due to additional injections of steam. If the option DROPOUT would not have been used, the atmosphere would probably be saturated during entire simulations.
Despite the supposedly adverse effect of the DROPOUT option on aerosol condensation, a very good agreement between measured and calculated wet aerosol concentrations in the test vessel atmosphere was obtained for tests K188, K186 and K187.

### 4. SAMPLE CALCULATIONS WITHOUT CONTAIN OPTION DROPOUT

Some calculations were also performed without the use of option DROPOUT. There was no significant difference in the calculated thermal hydraulic conditions. However, large differences occurred in the calculation of wet aerosol concentration, due to the modeling of dispersed liquid in the atmosphere. The following figures show the wet aerosol concentration for test K186 and K188. Apparently, the CONTAIN code reproduced more closely the aerosol behavior when option DROPOUT was used.

![Graph showing wet aerosol concentration for test K186 and K188](image)

**Test K186** Total wet aerosol concentration (compare with fig. 5.23a)
Test K188 Total wet aerosol concentration (compare with fig. 5.24a)
Investigation of uncertainties of the KAEVER Experiments

Influence of the Aerosol Injection on the Calculated Aerosol Results

As described in the specification of the ISP44 the aerosol injection was not well known. From mass balances and sedimentation measurements inside the vessel it was concluded that 50 to 60% of the produced aerosol settled already in the tubes from the aerosol generator to the vessel, and that the material entering the vessel contained a fraction of larger particles that settled rapidly during the injection phase. Since the measured data were too poor to evaluate reliable injection rates with the corresponding particle sizes the measured aerosol concentration and median diameter at the end of the injection were given as the starting point for the depletion phase of the calculations. The injection rates given in the specification based on calculations and should have served as a help to reach the starting point.

The uncertainties of the injection phase are investigated by parametric studies done with COCOSYS to the test K188. The base case (1) is the GRS calculation to the ISP44. It uses the given values for the injection rate, the number median diameter of 0.26 µm and the standard deviation of 1.45.
Figure 1: Investigation of the influence of the aerosol injection on the depletion phase. Aerosol concentrations: (1- solid line) base case, (2-dashed) four times larger aerosol mass, (3-dotted) four times larger aerosol mass and larger particle diameter.

In the calculation (2) the injection rate is increased by a factor of 4, representing the aerosol mass which is estimated to have entered the vessel in reality. The other parameters are the same, which however does not account for the fraction of larger particles mentioned above. This is “tried” in calculation (3) by using a mass median diameter of 3 µm and the injection rate of calculation (2). In figure 1 the calculated aerosol concentrations are shown. From 15 min after the first measurement point on they decay almost in parallel during the depletion phase. While the concentration of (3) comes close to that of (1) the concentration of (2) stays slightly higher. This shows, that uncertainties of the injection phase have some impact on the absolute aerosol concentration but have only a small influence on the depletion rate. This was taken into account in the evaluation of the ISP44 by giving most importance on the depletion rate.

Influence of the Steel Components Attached on the Vessel Outside (Structure 10)

External steel components like the door opening mechanisms were an important path of heat transfer from the vessel to the ambient. They acted like cooling fins. Since a calculation of the three dimensional heat flow in these components is almost impossible, they were simulated by
the additional “structure number 10”. The participants of the ISP44 were free to adjust the size of this structure, since it depends on the outside heat transfer coefficient used by the individual code. The impact of this simulation is investigated by two COCOSYS calculations. The base case is again the GRS calculation to the ISP44, which uses for structure 10 an area of ($A_{STR10}=\) 1.25 m$^2$. This is not much compared to the area of other not insulated wall of 4.6 m$^2$. In comparison to that the total wall area inclusive the insulated part was 30 m$^2$. In a parametric calculation $A_{STR10}$ was reduced to 0.8 m$^2$. These results in a higher pressure and a higher atmospheric temperature compared to the base case. While the base case simulates the atmospheric temperature almost exactly during the aerosol depletion phase the parametric calculation shows a 4 K higher temperature (fig. 2). The impact on the calculated aerosol concentrations however is so small that it can almost not be detected in (fig. 3). It is concluded that moderate deviations in thermal hydraulic conditions caused for example by the external steel components have only a minor influence.

Figure 2: Influence of the heat loss simulation, atmosphere temperatures of: (2) base case $A_{STR10} = 1.25$ m$^2$, (1) $A_{STR10} = 0.8$ m$^2$
Figure 3: Influence of the heat loss simulation, aerosol concentrations of: (2) base case $A_{STR10} = 1.25 \text{ m}^2$, (1) $A_{STR10} = 0.8 \text{ m}^2$

Fog Formation Test K156

The fog was measured with the Fast Aerosol Extinction Spectral Photometer (FASP). In the KAEVER test it was calibrated to the optical parameters of water droplets. In test K156 the fog formation was investigated. No aerosol material was injected which might have had an influence for example by steam condensation on hygroscopic particles or disturbance of the measurement signal by solid particles. First nitrogen was injected to increase the content of non-condensable gas, than steam was injected with a rate of 3.2 g/s. At 20 h the conditions were similar to those of KAEVER tests chosen for the ISP44 with partial pressures of 0.8 bar for steam and 2.1 for nitrogen and about the same steam injection rate. All the time fog was detected with a concentration of more than 10 g/m$^3$ at the beginning when the vessel was cold and 3 g/m$^3$ at 20 h when it was heated up. Then the injection was stopped and started again after some hours with a rate of 2.1 g/s. For the last phase however not all data are available.
Two calculations were done with the earlier version 1.1 of COCOSYS. The Kelvin effect was used. In calculation (1) the emissivity of the wall was input with 0.4 in (2) with 0.96. The lower heat radiation from the atmosphere to the wall in (1) results in a smaller volume condensation rate (fog formation rate) compared to (2), see figure 4.

Figure 4: Fog formation test K156, volume condensation rates, (1) emissivity of 0.4, (2) emissivity of 0.96.

The fog concentration is simulated well (fig. 5). According to the volume condensation rate case (1) shows lower values than (2). The calculations stopped near 15 h due to numerical problems caused by the Kelvin effect. (The volume condensation rate shown for the whole test in fig. 4 is the result of a calculation in which the Kelvin effect was turned off).

Important results are:

- In test K156 fog was detected all time without influence of aerosol material.
- The conditions at 20 h were close to the tests chosen for the ISP44.
- Since COCOSYS simulates well the fog formation in K156 it can be concluded that this is the case for the ISP44 tests, too.
Figure 5: Fog formation test K156, fog concentration, (1) emissivity of 0.4, (2) emissivity of 0.96
RUB/LEE Comments on the ISP 44 Calculations with the System Code COCOSYS

The computations of RUB/LEE in the frame of the ISP 44 very clearly show the capability of COCOSYS to simulate the phenomena dealt with in the KAEVER experiments under consideration. Here, the main challenge was not to investigate thermal hydraulics, but to predict the aerosol behavior of a three component aerosol in the frame of a “blind” calculation by COCOSYS. In advance additional post test computations, so called “open test calculations”, had been conducted in order to adjust model parameters in accordance with the requirements of the KAEVER facility. These open tests can be split into three experiments performed with single component and one with two component aerosols. With regard to the single component experiments, the components are chosen such that each component of the blind test is used once. Within the two component experiment two of the three components are considered.

The following list shows the main characteristics of the five experiments.

<table>
<thead>
<tr>
<th>Exp.</th>
<th>Components</th>
<th>Comments</th>
<th>Status</th>
</tr>
</thead>
<tbody>
<tr>
<td>K123</td>
<td>CsI</td>
<td>soluble aerosol, slightly superheated conditions</td>
<td>open</td>
</tr>
<tr>
<td>K148</td>
<td>Ag</td>
<td>insoluble aerosol, saturated conditions</td>
<td>open</td>
</tr>
<tr>
<td>K186</td>
<td>Ag, CsOH</td>
<td>insoluble and hygroscopic aerosols, saturated conditions</td>
<td>open</td>
</tr>
<tr>
<td>K188</td>
<td>CsOH</td>
<td>hygroscopic aerosol, saturated conditions</td>
<td>open</td>
</tr>
<tr>
<td>K187</td>
<td>Ag, CsI,CsOH</td>
<td>insoluble, soluble and hygroscopic aerosols, saturated conditions</td>
<td>blind</td>
</tr>
</tbody>
</table>

The results of the computations are for most of the test cases in a good agreement with the experimental results. Here, two deviations of the RUB/LEE open test calculations compared to
the experimental results shall be discussed only: In the simulation of experiment K148 for the 
ISP 44, the aerosol concentration was strongly overestimated and the computed pressure in the 
late Phase II of experiment K186 was significantly lower than the pressure in the experiment. 
RUB/LEE decided to perform additional simulations with modified input data sets. The changes 
for these reruns and some results are discussed in the following.

Rerun of Experiment K148

Several reruns of K148 have been performed subsequent to the ISP 44 workshop July 2001 in 
Cologne. Computations of K148 taking into account the Kelvin effect were generally more 
unstable than the ones without considering the Kelvin effect. The latter, in turn, lead to an 
unrealistic simulation of the Ag aerosol behavior because of the insoluble Ag is treated as a 
soluble aerosol. So a computation with Kelvin effect is needed to simulate the Ag aerosol 
behavior correctly.

Several parametric studies of numerical variables were performed to prepare a stable calculation 
with reasonable results. One decisive demand for these parametric studies was to use the given 
boundary conditions from the ISP specification and to change only the not specified variables. 
Within these parametric studies it was detected, that the variable NSTEP denoting the number of 
aerosol time steps for condensation on particles to reach the equilibrium state is important for 
the numerical stability of the code. With a value larger or equal to 10 the computations are more 
stable and a larger thermal hydraulics and aerosol time step can be used. With these changes 
the computation results for the experiment K148 become more realistic.

The dry aerosol concentration as a characteristic parameter for the aerosol behavior to illustrate 
the improvements of the additional post test calculation is shown in Fig. 1. The concentration 
peak in the injection phase in the experiment nearly is reached in the simulation and the 
decrease of the dry aerosol concentration in the depletion phase is also represented very well by 
COCOSYS.
Fig. 1 Dry aerosol concentration in experiment K148 and COCOSYS rerun.

**Rerun of Experiment K186**

In the case of experiment K186 it was decided to perform a rerun due to the pressure loss in the late test phase. The lower pressure in the simulation was caused by an error in the input data set. Along the whole Phase II nitrogen was removed from the test vessel at a constant value. This leads to a significant decrease of nitrogen mass in the simulation and consequently to a lower pressure.

Fig. 2 shows the pressure and temperature for the experiment K186 and the COCOSYS calculation. The appropriate values are in a good agreement. Nevertheless, the aerosol behavior has not been influenced much by the deviation of the pressure.
Fig. 2 Pressure and temperature in experiment K186 and COCOSYS rerun.

Finally, the results of the computations are now for all test cases in a good agreement with the experimental results. But nevertheless some minor deviations still appear in the calculation of the aerosol behavior. Especially the aerosol depletion in cases of soluble and hygroscopic aerosols is overestimated.
Post-Test Calculation of the Aerosol Experiment KAEVER 187 ISP 44

Jiri Dienstbier

Introduction

Repeated calculation of the ISP 44 KAEVER 187 experiment performed after the results of the blind calculation have been published is described in this short report. NRI Rez participated in ISP 44 due to limited manpower only partially, by solving the blind experiment KAEVER 187 using the recently installed version of MELCOR, MELCOR 1.8.5. The results have been submitted to GRS [1] and are included in the ISP 44 report [4].

The experiment was not completely blind, limited thermal hydraulic data measured during the experiment and aerosol concentration at selected time have been available. Comparing to them, the NRI results did not indicate major difference. After publishing the results of other participants of this exercise [4], it became, however, clear, that the NRI results match the measured thermal hydraulic behaviour worse than the others. Moreover, in the important regions of aerosol source and depletion, the effect of thermal hydraulic parameters on aerosol behaviour is very strong, because the conditions are close to 100 % humidity and a small deviation to the superheated conditions influences strongly aerosol behaviour. Though the aerosols results of different participants showed generally larger deviations and the NRI results were not exceptionally worse, the NRI results exhibited some strange features, like more flat top of the concentration curve in the source period.

For these reasons the calculations were repeated after a thorough input data analysis, the results are described here. The same code and code version, MELCOR 1.8.5, as for the blind calculation was used.
Short overview of the blind calculation features related to post-test calculation

For the blind calculation of the experiment, one control volume for the test vessel was used as in most other participant calculations. Other control volume with time constant parameters represented the environment. The control volume representing the vessel was specified with non-equilibrium between the atmosphere and the sump, which is also the MELCOR default.

Because of complications to model strictly the whole phase I, only phase II was modelled with the initial conditions that were specified in its beginning. The whole phase I was replaced by one hour period before phase II with constant thermodynamic parameters in the control volume to obtain better temperature profile in the wall. During a part of this period, the heating mats represented by internal heat source were also modelled.

As the code cannot model sections of cylindrical walls, it was decided to replace all of them by flat heat structures. The bottom of the control volume was modelled by more slanted walls and denser volume – altitude table was used to correctly describe the contact of water with the walls. Generally, the table of structures recommended by GRS for COCOSYS [2] was used. Insufficient cooling comparing to the experiment was observed in first calculations and also smaller non-equilibrium between the sump and the atmosphere than indicated in the experimental results. This was slightly improved by increasing the virtual wall area to 5 m$^2$ and adding another virtual wall of the area 2 m$^2$ to the sump. To correctly describe the aerosol behaviour, the virtual walls were extracted from the aerosol deposition areas. Finally a good agreement between the experiment description and the MELCOR model was reached.

The sources of steam and nitrogen were modelled according to description on the experimental data CD, they were replaced by mass and energy sources. The leak was modelled as a true leak, by a flow path with given size and other properties.

Aerosol sources have been specified also in agreement with the description of the experiment. The default class numbers from MELCOR 1.8.5 were used. More exactly all 16 classes were retained, but their source and initial mass was zero except of the three really used aerosols – CsI, CsOH, Ag. The possibility to re-normalize the source to the experimentally measured concentration in one time point was not used. The MELCOR 1.8.5 default size sections have been used, 10 sections from 0.1 µm to 50 µm particle geometrical diameter. All other aerosol parameters like shape factors were specified as recommended in [2] or on the CD. In case of
particle diameter, the specified volume median diameter (input as mass median diameter) was used for the sources. The code requires to input a constant aerosol particle density in time used for different materials. After verifying that soon after the aerosol injection there will be a massive condensation on the particles and a larger part of the aerosol mass will become water, the default density 1000 km/m^2 was preserved. The results showed little sensitivity to this parameter.

Using the code hygroscopic model led to extremely fast water condensation on the particles and their removal. Even though this was a blind calculation, comparison with the results of other ISP 44 non-blind experiments for soluble and insoluble aerosols [3] led to the idea that the results with hygroscopic model are wrong. For this reason, the hygroscopic model has been intentionally switched off.

More detailed description of the blind NRI calculation can be found in [1] or [4].

Findings when comparing the blind calculation results

When checking the thermal hydraulic results of the blind calculation with the experimental data, higher pressures and temperatures were observed in the calculated results, fig. 1, red curves. After checking other results, it became clear that this was caused by slightly higher heat removal from the experiment or in the calculation of other participants than in the MELCOR model used by NRI. The input was checked thoroughly and following corrections have been performed:

1. An error in the thickness of structure 7 (vessel vertical walls) was found and corrected. The correct thickness of this structure is 0.2 m while 0.25 m was erroneously defined in the blind calculation.

2. The 2 mm thickness of the sheets on the external insulation surfaces was subtracted from the insulation thickness.

3. Internal wall heat sources used in the initial period (modelling phase I of the experiment) to describe the heating mats were removed.

4. The initial period was extended from 1 to 2 hours to reach a more exact initial temperature profile in the walls.

5. The radiation length path for all inner and outer surfaces was extended from 0.1 m to 0.5 m.
6. Radiation heat transfer was added for the inner surfaces of the virtual walls.

7. The emissivity of the external zinc plated surfaces, which was said to be uncertain in the experiment, was increased from 0.25 to 0.6.

8. The bottom virtual structure area was extended from 2 to 5 m$^2$.

It is interesting, that most of these corrections had only negligible or small effect on the results. This is also true for 1) in spite of the relatively large area of this structure. The only exceptions, effective changes that strongly increased the heat removal, were 5), increasing the radiation length, which is physically reasonable and 8), increasing the virtual floor, which is somewhat artificial. It can be, however explained as an effort to compensate for the change from cylindrical geometry of the experiment to rectangular geometry of the calculation. Because the internal surfaces were generally conserved, the external ones are always decreased by this modelling.

After all these changes, the heat removal from the control volume increased and the pressure and temperature characteristics show a general cooling trend as observed in the experiment, fig. 1, black lines. There is also a visible impact on the aerosol sedimentation. The aerosol concentration curve in the atmosphere became less “flat”, fig. 2, this means that their deposition was faster. This can be explained in the slightly faster condensation of water on aerosols caused by slightly shorter period during the aerosol source when the atmosphere became slightly superheated. The atmosphere was supersaturated during the rest of the experiment, which the MELCOR code treats as 100 % humidity adding the extra water (fog) to the aerosols.

After checking the aerosol input one more time, a way was found how to compensate for the fact that constant particle density is required by MELCOR and the default 1000 kg/m$^3$ was used expecting high contribution of water while the aerosol source material density is much higher. The aerodynamic mass median diameter of the source particles, AMMD was calculated:

$$\text{AMMD} = \text{MMD} \times \sqrt{\frac{\rho_p}{\rho_{\text{water}}}}$$

where $\rho_p$ is the particle density of the source aerosols

The calculated AMMD was then input into the code as MMD. Though this improvement changed the aerosol results in the desired direction, the effect on the aerosol behaviour, e.g. the concentration curve in fig. 2 was much weaker than that caused by the changed thermal
hydraulic conditions and the change in atmosphere superheat discussed above. The black curves in fig. 2 already include this change in MMD.

**Conclusions**

After the changes described, the agreement of the results of thermal hydraulic and aerosol calculations with MELCOR 1.8.5 show acceptable agreement with the experimental ones and those of the other participants. It should be noted, however, that the solubility effect was neglected and all aerosols were considered as non-hygroscopic. In case of switching the model on, the same non-physical results were obtained as before. The physical explanation for obtaining physically reasonable results even without the hygroscopic model is the following. In an atmosphere close to saturation or even supersaturated, the water condensation on aerosols is very intensive which suppresses the solubility effect – the aerosols became mostly droplets of water. This is also the reason why this effect was week in KAEVER 187 with saturated atmosphere. For some reason, MELCOR 1.8.5 model does not respect this fact while it seems to work correctly in more superheated atmosphere. The growth of aerosols in saturated conditions then becomes strongly overestimated due to strong overestimation of the solubility effect in MELCOR and their deposition is very fast.

More improvement of the aerosol results could be also reached with better knowledge of the aerosol source intensity. When normalizing the results on the point after the aerosol injection, high normalization factors of 3 to 8 had to be used. The calculated aerosol concentration was much higher than the measured one and their coagulation might have been strongly influenced. This may explain the too fast depletion observed at the end of the aerosol period of the experiment, both in the blind and the post-test calculation, fig. 2.

**References**


Fig. 1 Pressure and temperature

ISP 44 ... KAEVER 187A ... post experiment calculation

MELCOR 1.8.5
Fig. 2 Dry aerosol mass concentration in the atmosphere MELCOR 1.8.5