COCOSYS

Short description

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Content

1 Objective and Structure of COCOSYS

The simulation of a severe accident propagation in containments of nuclear power plants is required for the analysis of the potential consequences of severe accidents and possible counter measures under conditions as realistic as possible. Therefore, at GRS the **Co**ntainment **Co**de **Sys**tem (COCOSYS) has been developed. The main objective is to provide a code system on the basis of mechanistic models for the comprehensive simulation of all relevant phenomena processes and plant states during severe accidents in the containment of light water reactors, also covering the design basis accidents.

In COCOSYS /ALL 05/ mechanistic models are used as far as possible for analyzing the physical-chemical processes in containments. Essential interactions between the individual processes, like e.g. between thermal hydraulics, hydrogen combustion as well as fission product and aerosol behaviour will be treated in an extensive way. With such a detailed approach, COCOSYS is not restricted to relevant individual severe accident phenomena, but will also make it possible to demonstrate the interactions between these phenomena as well as the overall behaviour of the containment. The structure of COCOSYS is shown in Fig. 1-1.

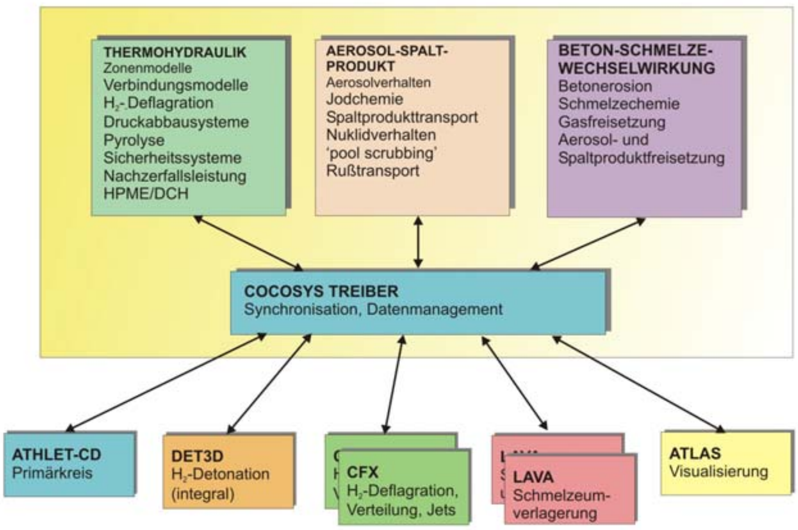


Fig. 1-1 Structure of COCOSYS

The complete system is divided into several so-called main modules. Each main module is a separately executable program, dedicated to one specific area of the overall problem. Communication among these main modules is effected via PVM /GEI 94/, which organises and controls the calculation sequence. The individual main modules calculate the overall problem in such a way that they can be coupled at time-step level, which means that the extent of the parameters that have to be exchanged is relatively low. To keep the complexity of the data exchange within reasonable limits, any data exchange is only allowed between the main modules and the COCOSYS driver. Due to the fact that the main modules are independent programs, undesired side-effects between the main modules are avoided, thus making maintenance of the overall system considerably easier. The use of PVM is a suitable basis for the parallelisation at the main module level. Apart from the three main modules THY (thermal hydraulics), AFP (aerosol fission product behaviour) and CCI (core melt behaviour) that belong to the inner part of the COCOSYS system, further programs are also coupled to COCOSYS, namely DET3D for the simulation of H_2 detonation (simplified coupling only), the commercial CFX code (a CFD program), and the in-house-developed LAVA code for the simulation of the spreading and dislocation of the melt. As regards the coupling, the overall concept in COCOSYS was modified in such a way that different modules can now run in parallel. Furthermore, different coupling variants (calculation of the width of the synchronisation intervals, data exchange) can be predefined by the COCOSYS user. The data can be visualised both online and offline with the ATLAS program. Some first experience is gathered with complete sequence calculations combining ATHLET-CD for reactor coolant circuit and core degradation processes and COCOSYS for containment ones.

1.1 Thermal Hydraulic

The **thermal hydraulic (THY)** main module is a so-called lumped-parameter model. The compartments of the considered power plant, test facility 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. To realize 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 (Fig. 1-2).

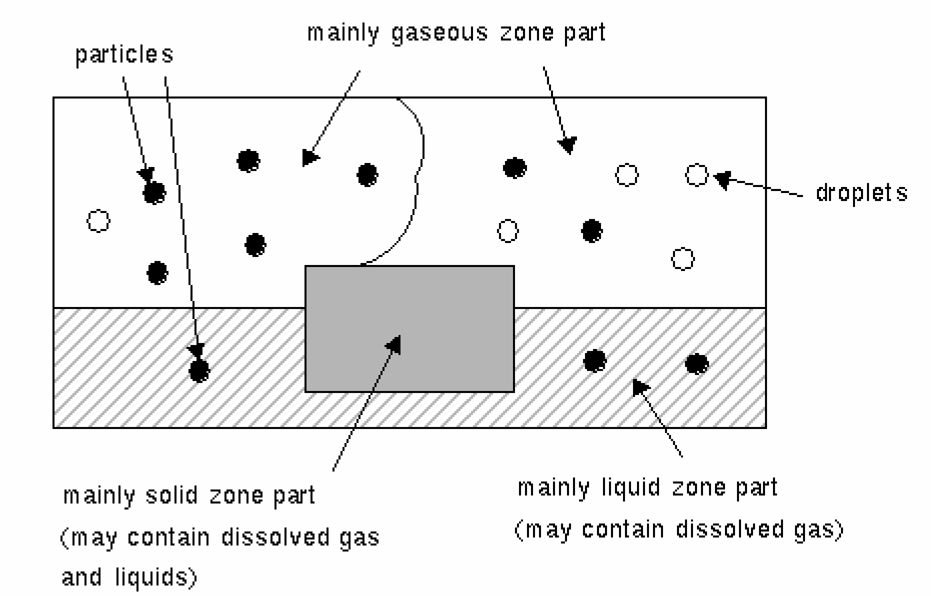


Fig. 1-2 Principle concept of zones

All zone related variables are based on this structure (components, zone parts, zones). All dimensions are defined by parameter statements. This leads to a transparent code structure for all implemented zone models.

Six different zone models are implemented in COCOSYS:

- **Equilibrium zone model**
  All components (liquid water, vapor and other non-condensable gases) are assumed to be mixed homogeneously, resulting in a homogeneous 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 behavior can be simulated.
- **Non-equilibrium zone model**
  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) correlations is possible. In case of a coupled THY-AFP simulation the deposition rates of fog droplets is based on the AFP calculation.
- **Hydrogen burning zone model (DECOR)**
  Due to the fact that the equations describing the flame propagation are directly depending on the thermodynamic gradient of the control volume, a special zone model based on the equilibrium zone model has been developed. Fig. 1-3 shows the principles of this model. DECOR is a one dimensional combustion model. Three burning axes can be defined by the user or by igniter locations to account for flame progression within a coordinate system established within the containment. During a deflagration process the zone is subdivided into an unburned and a burned zone part. The propagation of the flame results in a calculated burning velocity and a gas expansion behind the flame. All available flow connections and igniters have to be related to the burning axes to calculate the dynamic propagation of the flame.

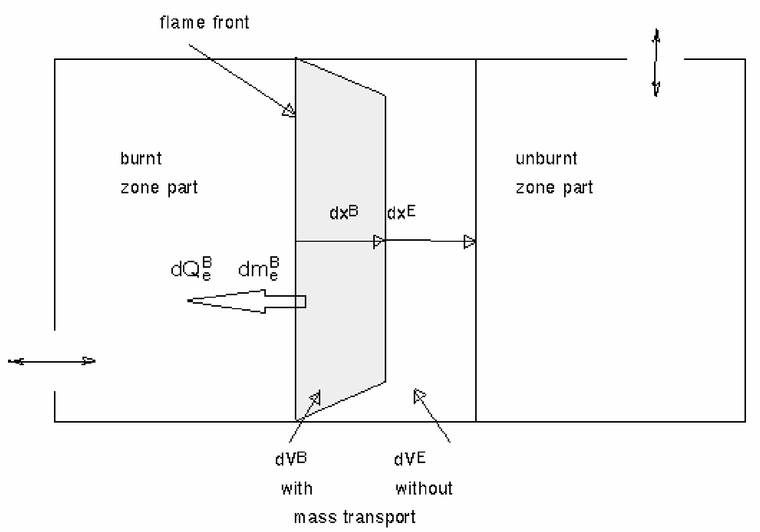


Fig. 1-3 Principle approach of the deflagration model DECOR

- **Pressure suppression zone model DRASYS**
  For the simulation of pressure suppression systems the DRASYS zone model can be used. The zone is subdivided into three zone parts: the pipe, the atmospheric part above the pool and the water pool zone part. DRASYS is able to simulate the dynamic pressure behavior resulting from the dynamics of the water level

in the pipe, the content of bubbles and condensation processes at the bubbles' surface. Fig. 1-4 shows the principle concept of DRASYS zone model.

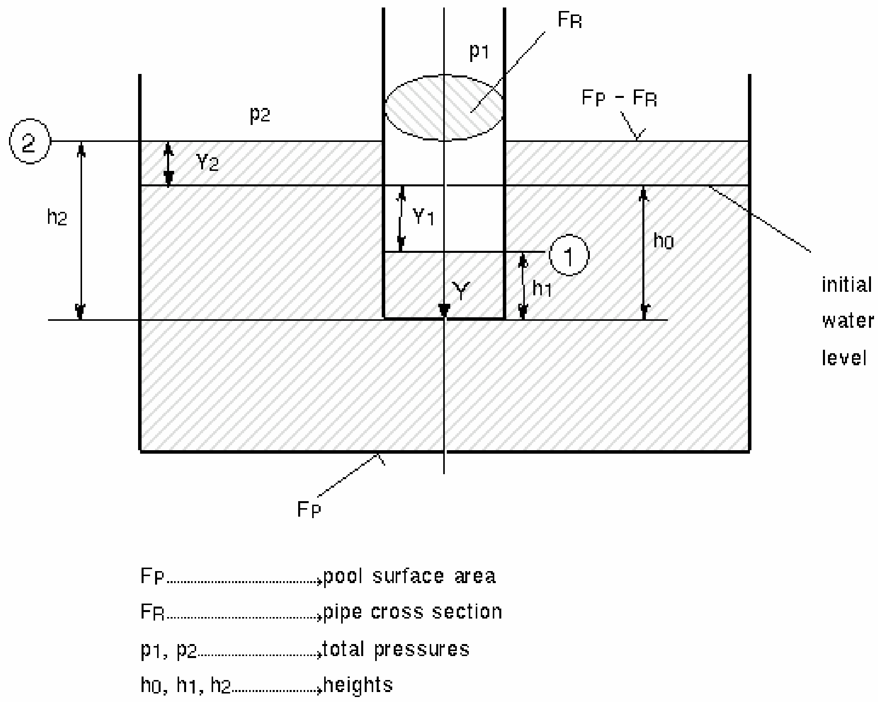


Fig. 1-4 Principle concept of the DRASYS zone model

- **VORTEX Condenser**
  The VORTEX zone model is designed for the description of dynamic processes in a jet vortex condenser (JVC) installed in NPP with VVER-440/230. A VORTEX zone is subdivided into four zone parts: downcomer or gas volume above the water (DC), vortex chamber or gas volume behind the water including gas volume of recirculation tank (VC), water pool (POOL) and water in the recirculation tank, if water exists there (RT). The thermodynamic state of the zone parts is calculated using the equations of the equilibrium zone model.
  In case of an accident with large mass and energy release from the primary or secondary circuits into the confinement, the pressure in the confinement rapidly increases. As result of this the JVC water is pushed from the downcomer through the jet nozzles into the vortex chamber. Passing the nozzles arranged under an attack angle of 45°, the water starts to swirl inside the vortex chamber. A vortex funnel creates, i.e. the water level in the downcomer simultaneously decreases whereas the level in the vortex chamber increases. When the water level at the periphery of the vortex chamber reaches its upper edge, the water starts to flood the recirculation tank and flows through recirculation pipes back into the pool inside the vortex chamber. The water swirling in the vortex chamber ensures an efficient condensation of the steam from the steam-gas mixture passing through the condenser. Non-condensable gases are directed via the outlet corridor to the environment.

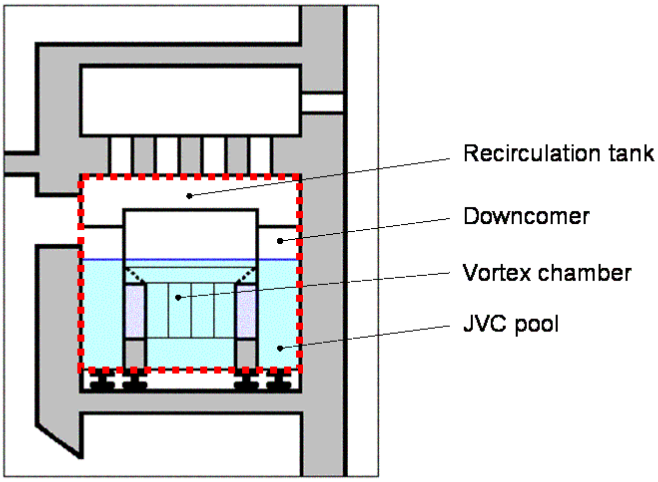


Fig. 1-5 VORTEX zone - model boundary and zone parts

- **Interface zone model**
  This kind of zone model has to be used for the coupling of COCOSYS with a CFD code (like CFX). The thermodynamic state variables needed are delivered by the connected CFD code. As described in the general zone concept, the zone control volume may be subdivided into several zone parts.

The **junction models** describe the flow interaction between different zones. In COCOSYS, the simulation of gas flow and water drainage is strongly separated, although water can be transported via atmospheric junctions by gas flow and dissolved gases can be transported via drain junctions. For an adequate simulation of the different systems or boundary conditions, specific junction models are implemented, like rupture discs, atmospheric valves, flaps/doors and specific pressure relief valves used in Russian types reactors. For the simulation of water drainage, several models are realised, describing the sump balance, water flow through pipes and along walls. The implemented pump system model is flexible enough to simulate complete cooling systems, e. g. emergency core cooling systems.

The walls, floors and ceilings of the considered building are represented by **structure objects**. The structure objects include all types of metallic and non metallic heat sinks within zones and between them. The heat flux calculation is one-dimensional, solving the Fourier equation. Plate-type as well as cylinder-type structures can be simulated. The whole wall (heat slab) can be subdivided into layers. Their thermodynamic state is defined by a layer temperature. The arrangement of layers can be chosen freely. Gaps inside a structure are possible, too. The heat exchange between structures and their assigned zones are calculated via convection, condensation or radiation (including wall-to-wall) heat transfer correlations. In these correlations, averaged properties (valid until 3000 °C) of the specified components are used. The initial temperature profile and the boundary conditions to the zones can be directly defined by the user.

To consider some effects along the flow path, **one dimensional junction** objects between zone volumes can be installed in the thermal hydraulic part of COCOSYS. Along the flow path the junction can be divided into several segments. Each segment may contain a structure between the inner gas segment volume and the surrounding zone volume or inner structure elements.

For the simulation of severe accident sequences and possible accident management measures it is necessary to take **safety systems** into account. In the THY main module it is possible to simulate different types of coolers (incl. atmosphere cooling system), spray systems, ventilation systems, ice condensers and catalytic recombiners. A special one-dimensional model was developed for passive autocatalytic recombiners (PARs), using an Arrhenius approach for the reaction on the catalytic surface. The recombination of CO is also calculated.

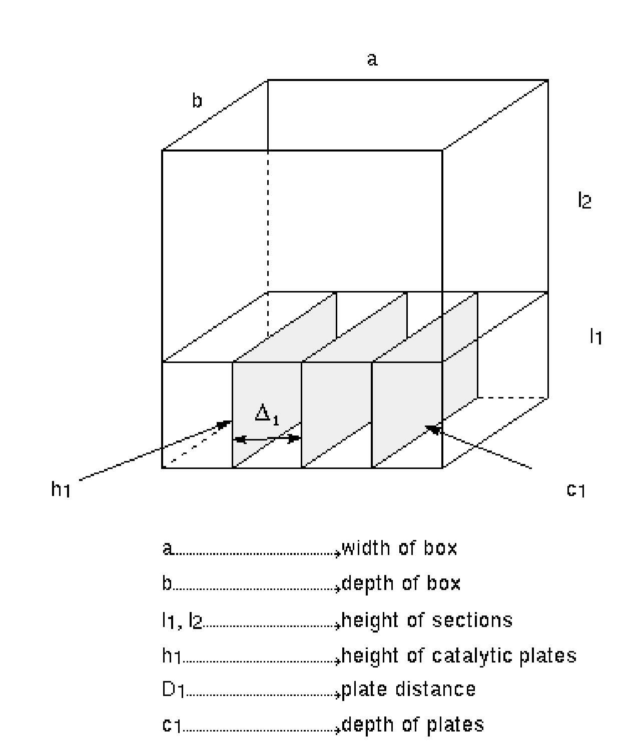


Fig. 1-6 Principle approach of catalytic boxtype recombiner (PAR)

The main thermal hydraulics module was extended to include the simulation of oil and cable fires. In the case of the oil fire, the burnt material is simulated by a structure with fixed temperature grid. For the calculation of the pyrolysis rate, a diffusion model is used which has been refined by application to different fire experiments. For the simulation of cable fires, a "simplified cable fire model" is available. This was tested on the HDR E42 experiments.

The thermal hydraulic part of COCOSYS uses the integration package FTRIX/FEBE /HOF 81/ which is an implicit Euler forward Euler backward integration solver. The network (of differential equation) concept in this part is written very general. Using special system routines it is relatively simple to introduce equations for new models.

1.2 Aerosols, Iodine and Fission Products

The **aerosol-fission-product (AFP)** main module is used for best-estimate simulations of the fission product behaviour in the containment of LWRs. Both the thermal hydraulic (THY) and the aerosol-fission-product (AFP) main modules consider the interactions between the thermal hydraulics and aerosol fission product behaviour. There is a distinction in COCOSYS in the simulation of aerosol particles, radioactive fission products and the iodine chemistry, i.e. they are simulated by different models.

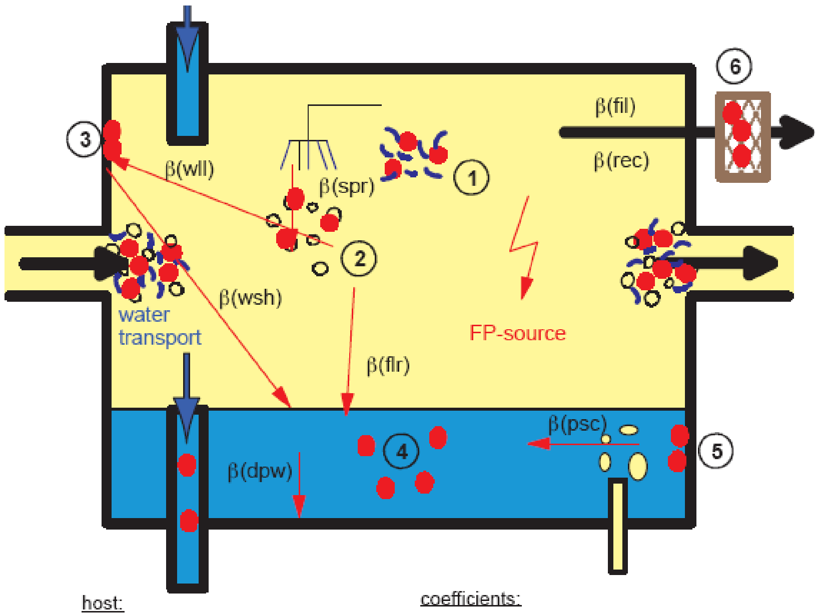
In the AFP main module of COCOSYS, the aerosol behaviour (**AERIKA**) of up to eight chemically different aerosol components is calculated with consideration of the thermal hydraulic boundary conditions. The module differentiates between soluble and insoluble as well as hygroscopic and non-hygroscopic aerosols. The following deposition processes are covered: sedimentation, diffusive deposition, thermophoresis and diffusiophoresis. For the calculation of the condensation on the aerosols, the moving-grid method MGA is applied which reduces the numeric diffusion between the size categories considerably. In the case of hygroscopic aerosols, condensation may already occur under superheated conditions and can change the level of humidity in the atmosphere. This repercussion on the state of saturation is taken into account in the thermal hydraulic calculation as the aerosol behaviour close to saturation depends highly on the degree of saturation.

The **FIPHOST** module calculates the transport of the fission products within the containment. The fission products are treated as the radioactive part of the aerosol particles and the radioactive non-condensable gases, whereas their mass is not considered in the model. FIPHOST differentiates between the atmosphere, the aerosol and the sump water as fission product carriers (5 host concept, see Fig. 1-7). The fission products can be deposited on surfaces in the atmosphere and in the sump. Their transport takes place according to the prevailing gas and water mass flows. All relevant processes relating to the fission products and the different carriers are considered: deposition of aerosol particles by natural processes or aided by technical systems such as filters and spray systems, washing-off from walls, and carrier change due to radioactive decay. Nuclide behaviour is simulated with the help of the **FIPISO** module. FIPISO considers the reactor's initial core inventory (pre-calculated by other codes) and calculates on this basis the decay of the fission products according to the time of the onset of the release by using established nuclide libraries (analogous to ORIGIN). Nuclide transport is calculated by FIPHOST. Generally, between 400 and 600 different nuclides are considered in the calculation. The decay energy in the individual zones and on the individual carriers is taken into account in the THY main module.

The chemistry in the **AIM** iodine module /WEB 06/ is based on IMPAIR and contains approx. 70 different reactions. AIM distinguishes between 17 iodine species in the atmosphere and 14 iodine species in the sump. It calculates iodine transport between atmosphere and sump as well as across the compartments. The behaviour of the aerosol iodine species CsI and AgI is calculated directly by the aerosol model in AFP. The AIM iodine module was tested on various ThAI experiments. This helped in particular to improve the interactions of I_2 on steel surfaces. Recently, AIM has been successfully used for the recalculation of experiments in connection with the ISP-41.

The retention of aerosols during gas transport through water pools is calculated by the SPARC-B module. This allows among other things the simulation of "pool scrubbing" in the pressure suppression system of a boiling water reactor.

There are special models for the simulation of filters (HEPA filters, granulate filters) implemented in COCOSYS. These also consider the increasing pressure loss in the atmospheric junctions.



host:
1 – gas
2 – aerosol
3 – gas phase surfaces
4 – water
5 – water phase surfaces
6 – systems (filter, recombiner)

coefficients:
β(flr) – deposition on floor
β(wll) – deposition on wall/ceiling
β(spr) – spraying
β(psc) – pool scrubbing
β(wsh) – washing
β(dpw) – deposition in water
β(fil+rec) – decontamination in systems

Fig. 1-7 FIPHOST control volume, fission product hosts

1.3 Behavior of Corium and Concrete

In case of a reactor vessel failure during a severe accident, the molten core would drop onto the concrete base structure of the reactor building. The interaction of the core melt with concrete would continue for a long period of time. During this, a number of phenomena are important for the subsequent course of the accident:

- concrete decomposition,
- release of steam and gases from the decomposing concrete,
- chemical reactions of these gases and of the molten concrete constituents with metallic constituents of the melt and within the containment atmosphere,
- dilution of the molten fuel materials by molten concrete constituents and alteration of the freezing behavior of the molten pool,
- aerosol and fission product release.

The COCOSYS **core concrete interaction (CCI)** main module is based on a modified version of WECHSL. The original application of WECHSL /FOI 95/, from which the GRS-code **WEX** /LAN 02/ is evolved, was given by calculations for the BETA test series, performed at Forschungszentrum Karlsruhe, so the models were oriented to the specific phenomenology of the BETA tests. WECHSL is in use for severe accident analysis of water cooled reactors for more than 15 years now. A number of further improvements and bug fixing has been realised at GRS. These improvements have led to the new version

WEX, which is not only available as a stand-alone code but also as part of COCOSYS and ASTEC V1.

WEX is a lumped parameter model for the analysis of the thermal and chemical interaction of reactor materials with concrete in a two-dimensional axis-symmetric concrete cavity. The model performs calculations from the time of initial contact of a hot molten pool with concrete until long-term basement erosion causing possibly a basement melt-through.

WEX considers either one oxide layer, which can contain a homogeneously dispersed metallic phase, or a separation of the molten pool into metal and oxide layers. Internal energy release is considered in form of decay heat or by exothermic chemical reactions. Energy is transferred to the melting concrete (ablation heat flux) and to the upper containment (thermal radiation or evaporation of sump water possibly flooding the surface of the melt). Gases generated during concrete decomposition pass through the melt. Water vapor and carbon dioxide are reduced as they pass through the metallic layer. Heat transfer between the molten layers is considered. For the heat transfer from the melt to the concrete a film model, a discrete bubble model or a transition boiling model is used, depending on the existing gas flow and on the inclination of the interface. The bulk of each layer of the melt is assumed to be isothermal with boundary layers at the interfaces. During cooling of the melt transient crust formation is modeled. Crusts are assumed to be permeable to gases. Solidus and liquidus temperatures for the oxidic phase are determined from a quasi-binary phase diagram. The relevant chemical reactions are formulated by gross reaction equations. The reactions are calculated within each time interval with the equilibrium concentration of the products achieved completely. The reactions are assumed to proceed in the order Zr, Si, Cr, Fe, so that Fe is oxidized only when all available amounts of Zr, Si and Cr have been consumed.

The current limitations of the code are the restriction to axis-symmetric geometries of the cavity and to either a homogeneous pool configuration or a layered pool situation consisting of an oxide layer on top of a metal layer.

For a very detailed consideration of the chemical processes in the melt (mixed or separated option) and the gas, aerosol and fission product release the **XACCI** module has been developed. This module uses the equilibrium thermo chemical model ChemApp /GTT 98/. Corresponding to the WEX programme two options exist for the simulation of the melt

- two phases - the oxide material is over the metallic phase,
- one mixed phase.

The XACCI module calculates for each phase and for the atmosphere above the melt the equilibrium conditions for the chemical components. Based on these results the mass and energy release including aerosol and fission products is calculated.

2 Status of Validation

According to the long tradition of investigations in the field of containment research in Germany COCOSYS is validated on a wide spectrum of tests performed in German or international test facilities. The tests performed in the former Battelle Model Containment (BMC) and the former Heiß-Dampf-Reaktor (HDR) as well as the ongoing tests in the ThAI facility form the backbone of the COCOSYS validation. The impressive validation status is summarized in Tab. 2-1.

Most of the older tests are calculated knowing the experimental results, whereas a large part of the recent calculations are performed without any knowledge about the experimental results. GRS believes that the predictive capability of a code and its user can only be demonstrated with so-called 'blind calculations'.

In such calculations the user has to select the options available in the code. In blind calculations this selection is based on the user's experience and the quality of the activated models inside the code.

Tab. 2-1 Experimental tests being used for COCOSYS validation

Thermal hydraulics	BMC	Rx4, C13, D3, D6, D7, FIPLOC-F2, VANAM M2*, M3, M4
	HDR	T31.3, T31.5, E11.1, E11.4
	ThAI	TH1, TH2, TH5, TH7, TH9, TH10, J10, TH13 (step 2 of ISP-47)
	TOSQAN / MISTRA	ISP-47 step 1 tests, MICOCO
Hydrogen combustion	BMC	Ix2, Ix7, Ix9, Ix23, Hx26
	HDR	E12.3.2
	NUPEC [D)]	B-2-6, B-8-3
Passive Autocatalytic Recombiner	BMC	Gx4
	HDR	E11.8.1
Spray systems	BMC	PACOS Px1
	HDR	E11.1
	NUPEC	M7-1
Passive systems / hydrodynamic	PANDA	BC3, BC4, PC1, ISP-42 tests, A, D, E and F
	BC-V213	LB LOCA test 1, SLB-G02
	GKSS	M1
Jets and plumes	BMC	HYJET Jx2
	PANDA	OECD-SETH T9, T9bis, T17
Pyrolysis [D)]	HDR	E41.7, E42
	NIST	more than ten tests of ICFMP No. 3
	OSKAR	ICFMP No. 4: tests T1 and T3
Aerosol behaviour	BMC	VANAM M2*, M3 (ISP-37), M4

	KAEVER	more than ten tests incl. ISP-44
Iodine chemistry	RTF	ACE 3B, PHEBUS 3 and 5 ISP-41 tests: P0T2, P1T1, PHEBUS 1
Iodine transport behaviour	CAIMAN	ISP-41 tests: 97/02, 01/01
	ThAI	J6, 8, 10, 11, 12, 15, 16, 17
Pool scrubbing		EPRI-II series 1 POSEIDON test series
Molten corium-concrete interaction (mostly performed in stand-alone mode)	BETA	V1.8, V3.3, V5.1, V5.2
	ANL	ACE L1, L2, L5, L8 MACE M3B, M4 OECD-MCCI CCI-2, CCI-3
	COMET	L1
Melt spreading	KATS	Tests No. 7, 14, 15, 17 and ECOKATS V1 and 1
	COMAS	Tests No. 5a, EU2b, EU3a, EU4
	VULCANO	VE-U7, VE-U8

D) performed by the developer himself and not by an independent person as required in the COCOSYS quality assurance procedure

2.1 Validation on HDR E11.4 Experiment

The validation of the HDR E11.4 experiment shows a very good agreement between the measurements and the calculation over a time schedule of 2 days. In this experiment the accident sequence of a ND case according to the German Risk Study Phase B /GRS 90/ has been simulated. After a long heat up phase hydrogen is released in the lower part of the containment. Additional the effects of sump heating and outer spraying have been tested. For the simulation the HDR containment (Fig. 2-1) has been subdivided into 92 control volumes. The Fig. 2-2 and Fig. 2-3 show some results. The red curves are the calculated results and the black curves are the measurement data.

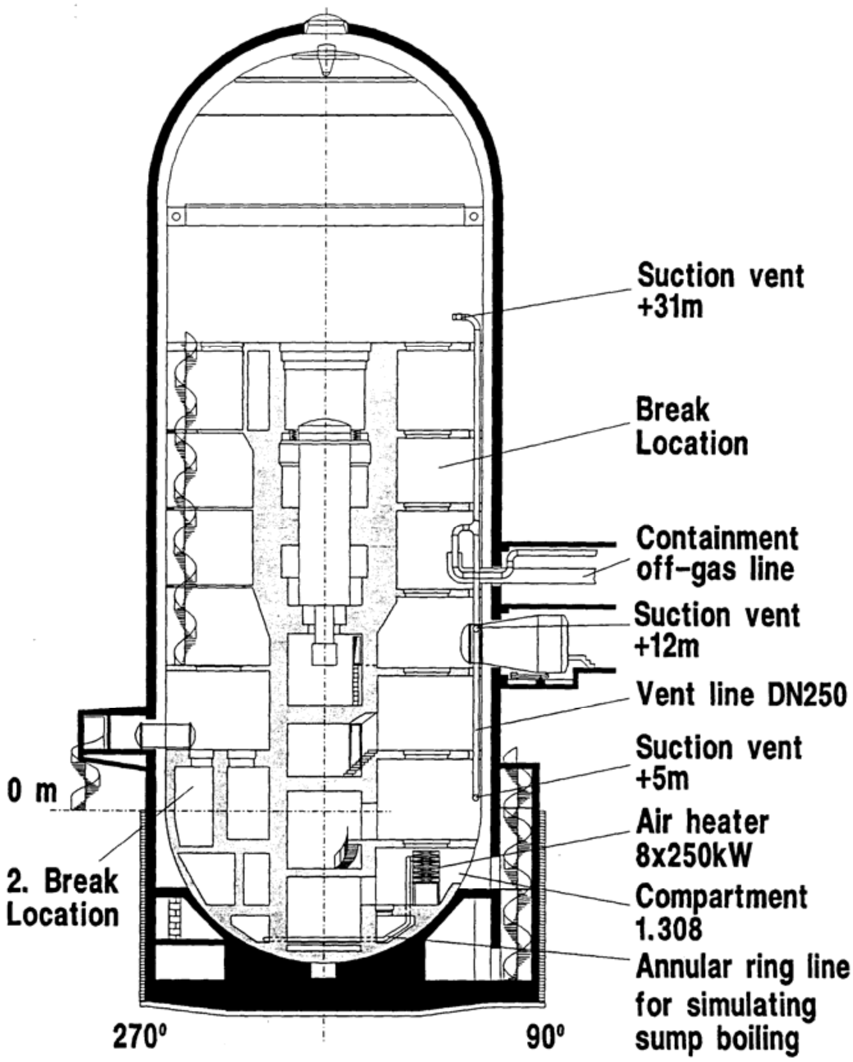


Fig. 2-1 HDR containment

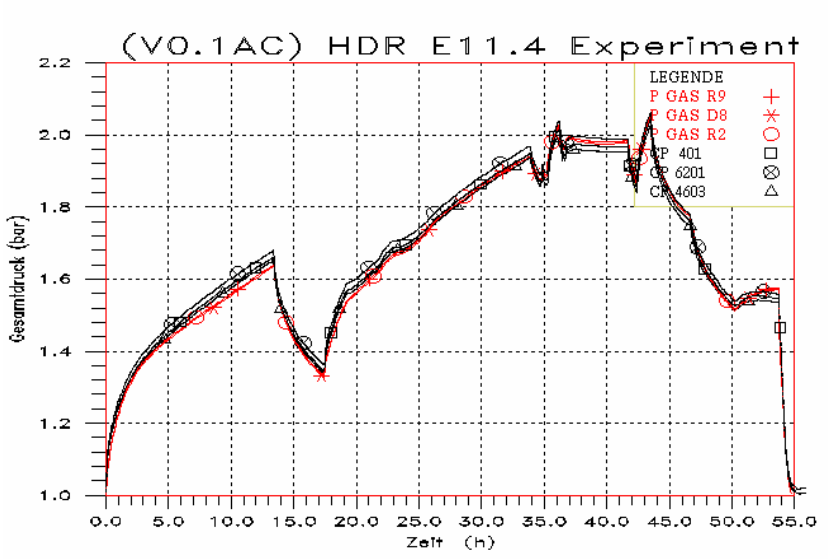


Fig. 2-2 E11.4 experiment, comparison of total pressure

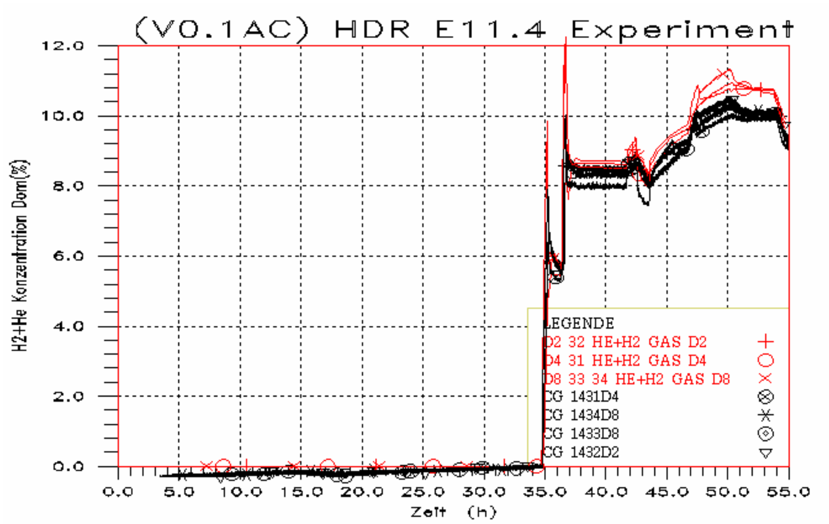


Fig. 2-3 E11.4 experiment, He+H2 concentration in the dome region

2.2 ISP-47 Step 2 ThAI

The prediction of the steam, hydrogen and air distribution is a main issue of the OECD International Standard problem ISP-47 /ALL 07, VEN 03/. Experiments with helium representing hydrogen have been performed in two French facilities, TOSQAN and MISTRA, and in the German ThAI facility. These experiments have been simulated numerically by several LP- and CFD-codes in order to validate them for reactor containment applications. This chapter focuses on the comparison between the experimental results of ThAI and the blind GRS prediction done with COCOSYS /FIS 05/.

2.2.1 Experiment

For this exercise the ThAI test facility is used in multi-compartment geometry established by inner structures. Inside a cylinder with a diameter of 1.4 m there is the central room. A middle floor consisting of 4 sections divides the annulus into an upper and a lower part by blocking 2/3 of the horizontal flow area (Fig. 2-4). The ISP-47 experiment started with atmospheric conditions (air at 20 °C). It lasted 7000 s and consisted of 4 subsequent phases.

The 4 phases of the ThAI ISP-47 experiment:

- A free upward directed helium jet was injected into the upper annulus, creating an air-helium cloud above the injection position.
- The injection position was changed to the opposite side of the upper annulus and a free upward directed steam jet was injected creating an air-helium-steam cloud in the upper plenum and the upper annulus.
- A horizontal steam jet was injected into the lower plenum. It homogenized the atmosphere up to the elevation of about 7 m, which is the lower third of the upper plenum. Above 7 m the helium concentration stayed higher than in the rest of the facility.
- In the last phase there was no injection. The stratification stayed the same as at the end of phase 3.

2.2.2 COCOSYS Simulation

The COCOSYS nodalisation (Fig. 2-5) subdivided the vessel into 52 zones forming 16 vertical levels. The zones are interconnected by junctions having a flow area according the geometry. The arrangement of the zones in horizontal direction allows the code to calculate either stratified atmospheric conditions or mixing of the atmosphere by a convection loop. The atmosphere entrainment by the upper injections requires a special simulation. The helium jet which becomes a buoyant plume after a short distance is simulated by zones forming a cone with an angle of 20°, according the jet theory. These zones are interconnected to each other and to the surrounding zones by junctions with flow areas according the geometry. The entrainment by the steam jet which enters the vessel with a velocity of 30 m/s and reaches its top with 2 m/s is calculated by an analytical formula. The lower horizontal steam injection is distributed to 75 % into the central zone below the inner cylinder and 25 % into the adjacent annulus node, bases on the formula. The walls of the vessel inclusive their insulation are simulated by heat structures.

The most important outcome of the ISP-47 has been atmospheric stratifications and the spatial distribution of the helium.

In phase 1 of the experiment the He-concentration increases in the upper plenum at 7.7 m (Fig. 2-6) due to the injection. It remains high for the rest of the experiment. Almost no He reaches the lower plenum until the start of the lower steam injection in phase 3 at 4600 s. Then the vessel atmosphere is mixed gradually as shown by the increase of the He content in the lower plenum at 1.6 m. At the end of phase 3 (5600 s) the atmosphere is homogenized except for the upper part of the vessel where the He concentrations remain high (Fig. 2-7)

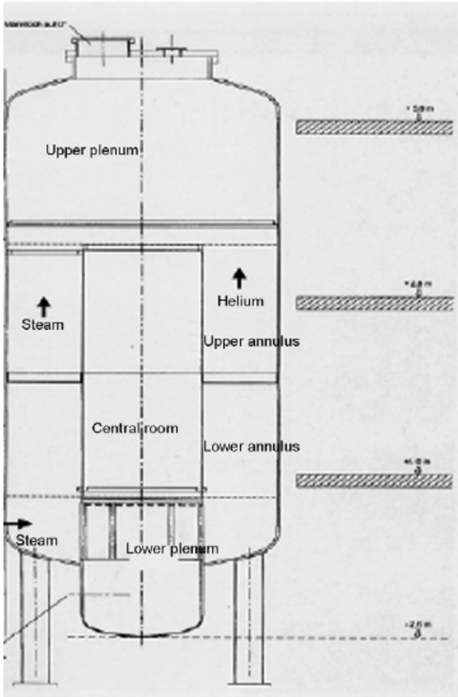


Fig. 2-4 ThAI test facility in the ISP-47 configuration

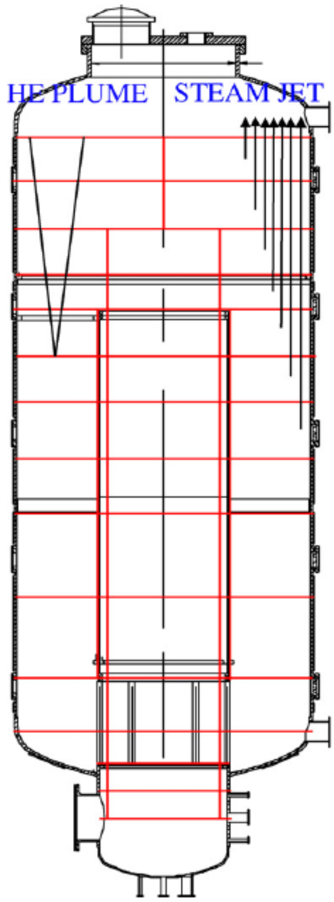


Fig. 2-5 COCOSYS nodalisation of ThAI ISP-47

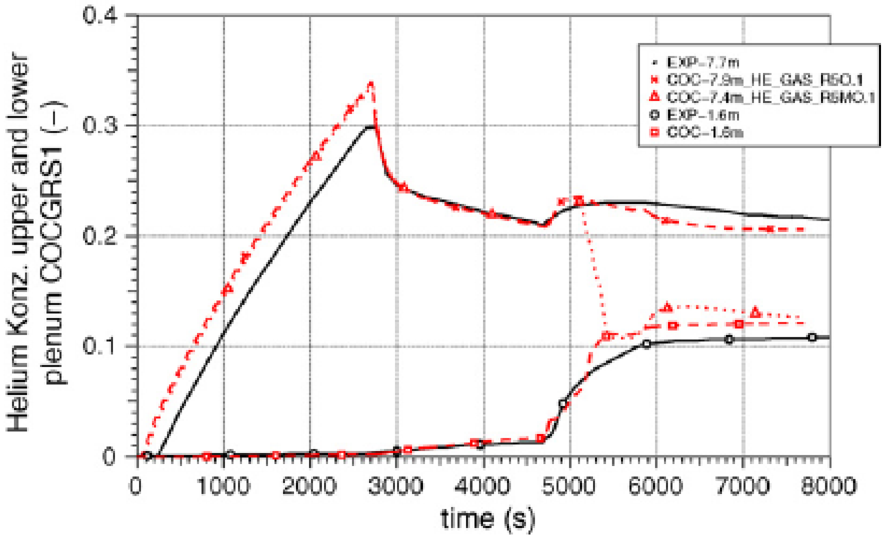


Fig. 2-6 Helium concentrations in the upper and lower plenum

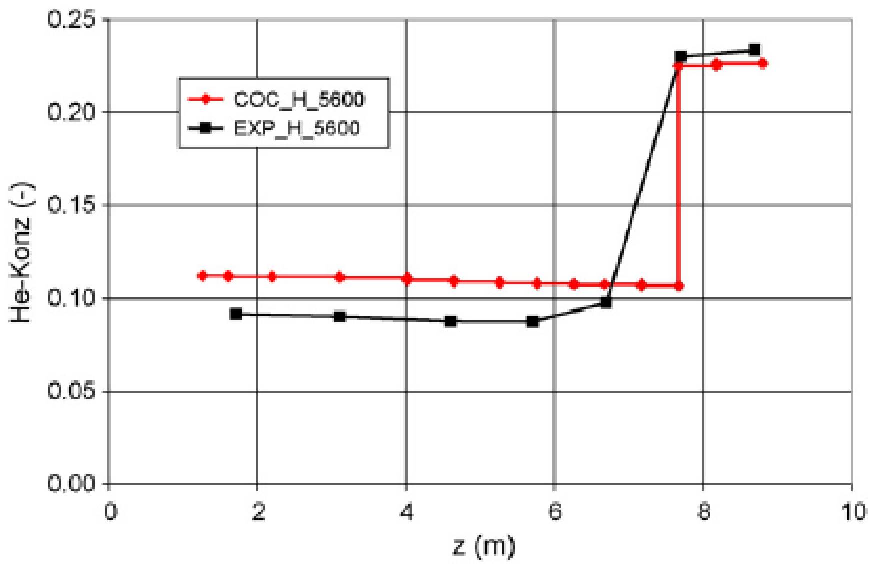


Fig. 2-7 Vertical Helium distribution at 5600 s

2.3 Validation on BMC VANAM-M3 Experiment

The Battelle model containment has a free volume of 626 m^3. It is build rotationally symmetric of reinforced concrete and is subdivided into several compartments. The VANAM test geometry (Fig. 2-8) represents roughly a PWR-containment. The following locations are provided for injections:

- Compartment R5 for the injection of steam or aerosol, respectively, suspended in a steam-air mixture.

- Compartment R3 for the injection of steam or the re-injection of air, respectively (the latter only during the heat-up phase).
- Annulus R9 bottom for the removal and re-injection of air during the heat-up phase.

Steam condenses at the containment structures. The condensate flows down into the sumps. Individual compartment sumps can form in R3, R4, R5, R6, R7, R8 and R9 each. During the phase 1 of the experiment sump water was drawn out of R9.4 (lower part of annulus).

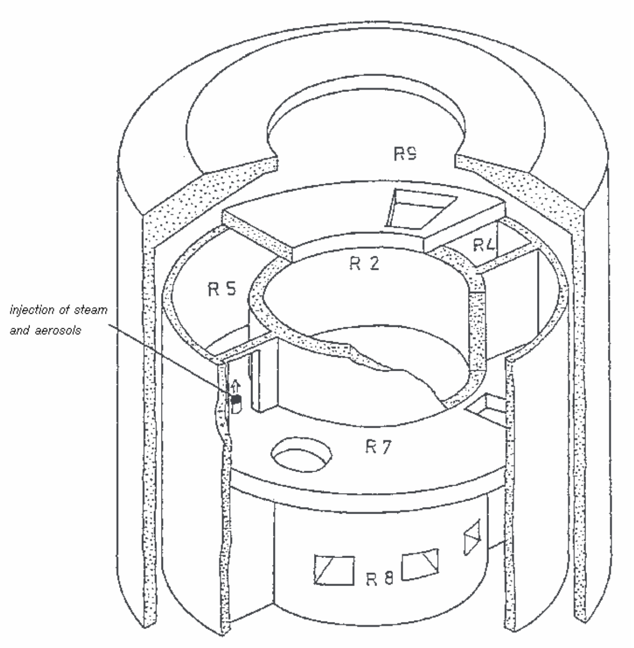


Fig. 2-8 Battelle Model containment

The Fig. 2-9 to Fig. 2-11 show some comparisons between the calculation (blue) and the measurement (black).

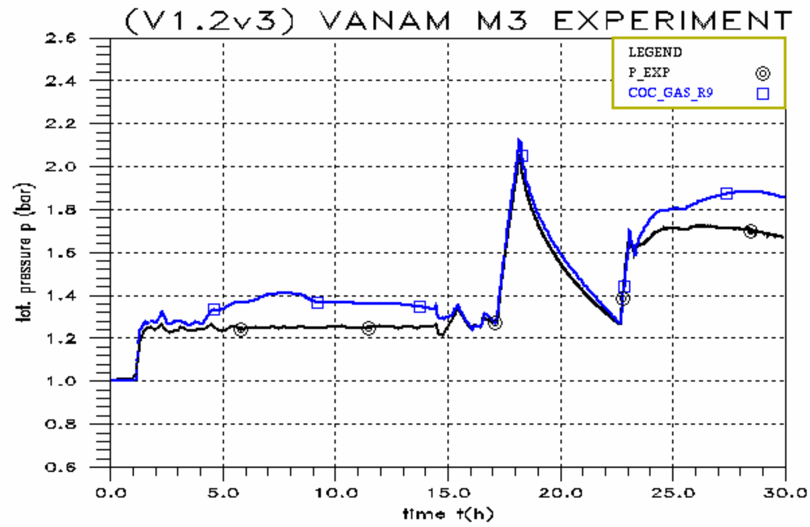


Fig. 2-9 BMC VANAM-M3 experiment, total pressure

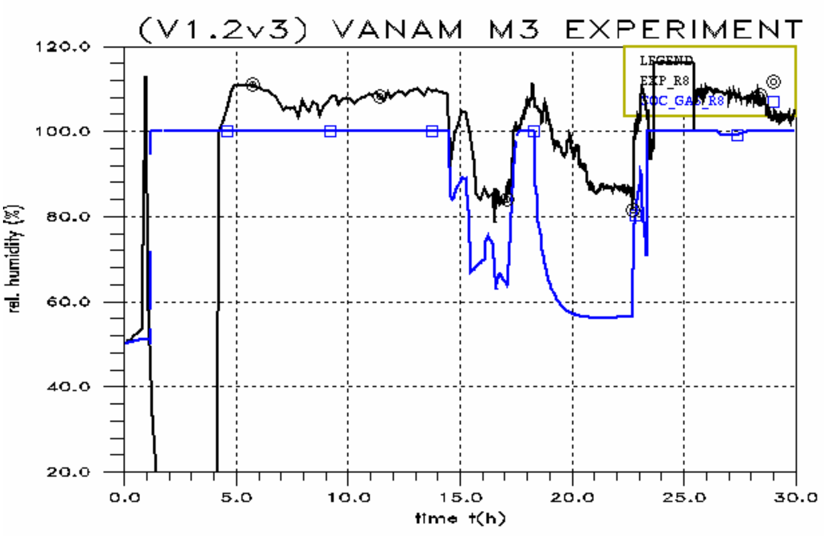


Fig. 2-10 BMC VANAM-M3 experiment, humidity in the dome R9

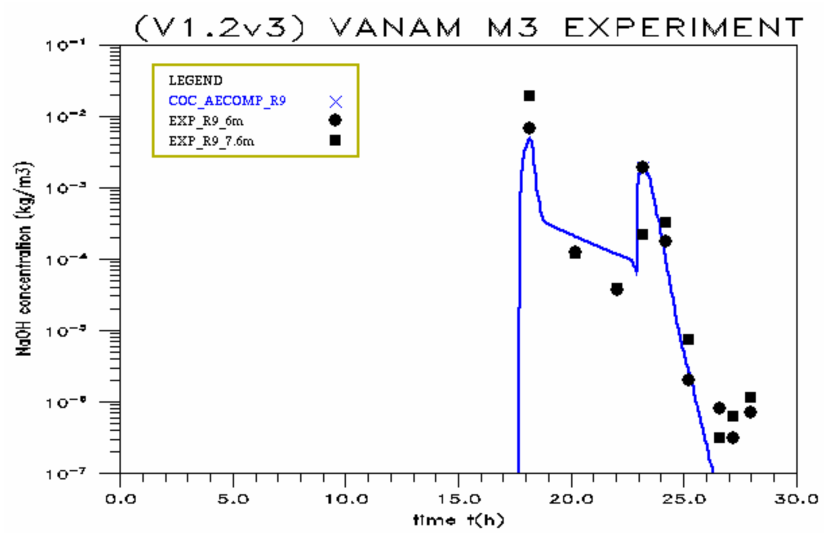


Fig. 2-11 BMC VANAM-M3 experiment, aerosol concentration in the dome

2.4 Multi-compartment Iodine ThAI Tests

The various iodine species in the gas phase of a reactor containment have a very different physical behaviour. Organic iodine is a non-reactive gas, caesium iodide and iodate are water-soluble aerosols and elemental iodine is a reactive gas. The time-dependent distribution and the deposition behaviour of these species are subject to a strong interaction with thermal hydraulics and the core melt aerosol. In COCOSYS, these interactions have been taken into account by a close numerical coupling of the iodine model AIM (Advanced Iodine Model) /WEB 06/ to the thermal hydraulics and aerosol module. In this way, the iodine transport in the containment, the local deposition on surfaces and the distribution between gas and aqueous phase can be simulated in detail.

The ThAI iodine experiments /FUN 04, WEB 06/ aim to fission product transport, depletion and resuspension processes in combination with thermal hydraulic phenomena. Fig. 2-12 depicts the coupling of thermal hydraulics and iodine effects in a typical iodine experiment. It becomes evident that for an adequate simulation of the iodine behaviour in the containment not only iodine chemistry is required, but at least to the same extent the different transport processes.

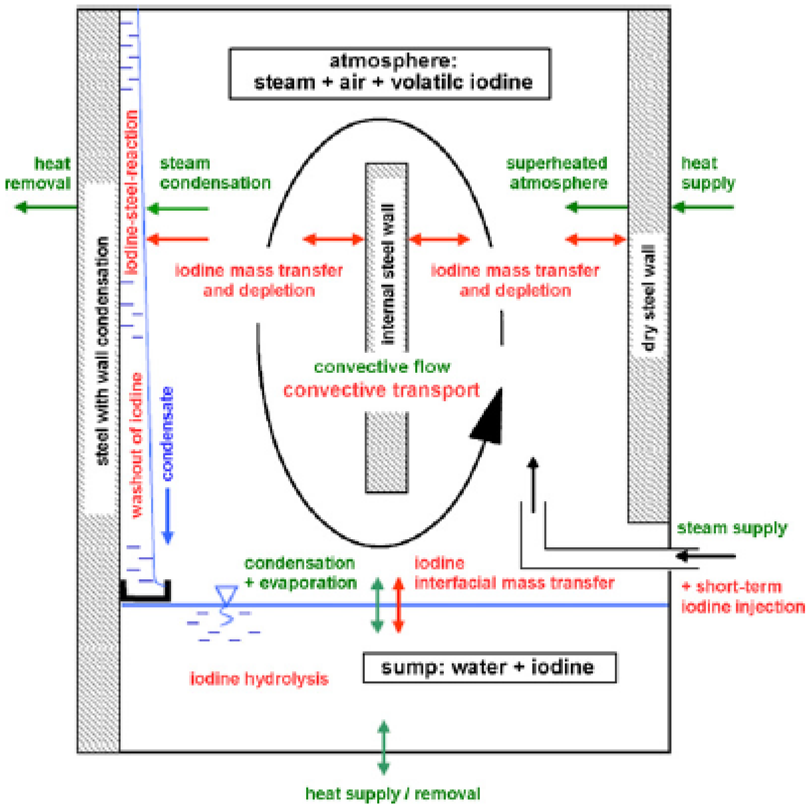


Fig. 2-12 Coupled thermal hydraulic and iodine phenomena investigated in a typical ThAI experiment

In order to generate a database for the validation of the iodine multi-compartment behaviour with COCOSYS GRS initiated iodine multi-compartment tests in ThAI. Due to its objective and the considerable vessel size as well as the controlled operation mode, the ThAI iodine multi-compartment experiments are unique in the world.

The Iod-10 and Iod-11 tests were performed under dry conditions, i. e. without wall condensation, whereas Iod-12 was performed with wall condensation. There operation mode shows essential elements of a core melt accident scenario in a LWR containment /WEB 06/. In the following, only test Iod-11 will be described as a typical example for the three tests.

2.4.1 ThAI Multi-compartment Iodine Test Iod-11

For the multi-compartment test Iod-11, the vessel was subdivided into five compartments: bottom compartment with main sump, lower annulus, upper annulus, central compartment and dome compartment (Fig. 2-13). In Iod-11 the lateral water tray was not filled. These compartments were atmospherically connected via openings. A thermally stratified, stable vessel atmosphere was built up by controlled heating of the upper vessel area. After that, about 1 g of elemental iodine was injected into the hot dome compartment. The concentration of the elemental iodine injected (I_2), which was labelled with the radioactive isotope I-123, was measured in the gas phase, in the sumps, in the wall condensate and as deposits on the dry steel walls. The six measuring positions of the gas scrubbers, which serve to measure the I_2 in the gas phase, allow a good spatial resolution of the iodine distribution in the vessel.

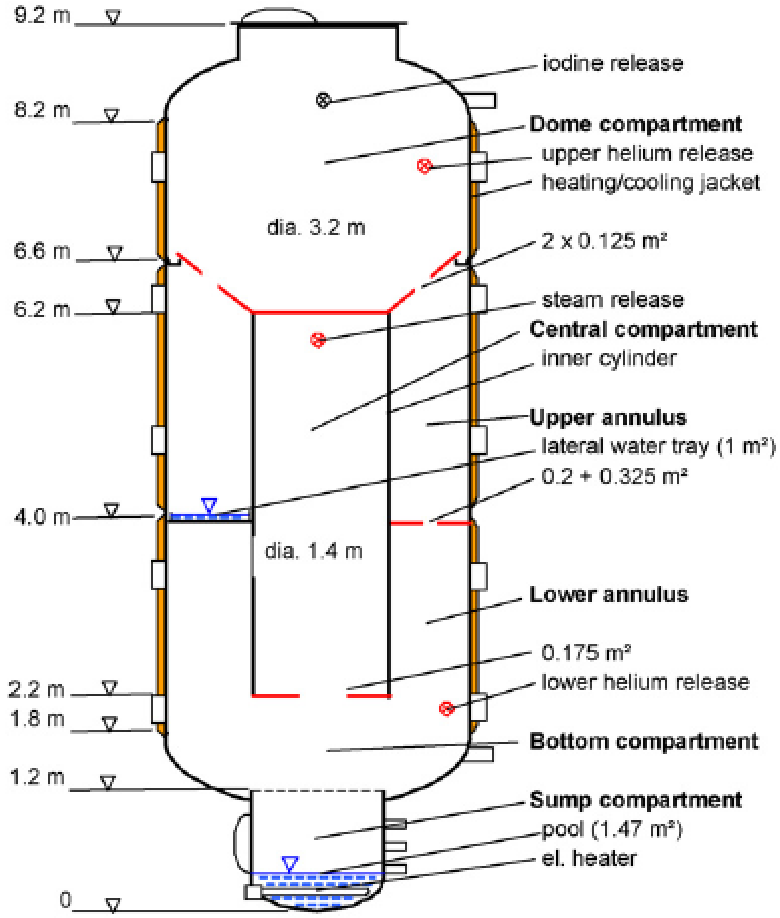


Fig. 2-13 Multi-compartment geometry of the ThAI vessel

In the Iod-11 test, the atmospheric stratification was broken up after a test duration of 4.5 hours by heating the lower and middle jackets and injection of light gas helium (He) into the bottom compartment. This caused a convection flow which distributed the gaseous I_2 not yet deposited on the dry steel walls in the entire vessel. The I_2-concentration in the dome decreased slowly and consequently a part of the deposited I_2 was resuspended. The wall served as an intermediate storage for I_2. Fig. 2-14 shows the measured iodine concentrations in the gas phase.

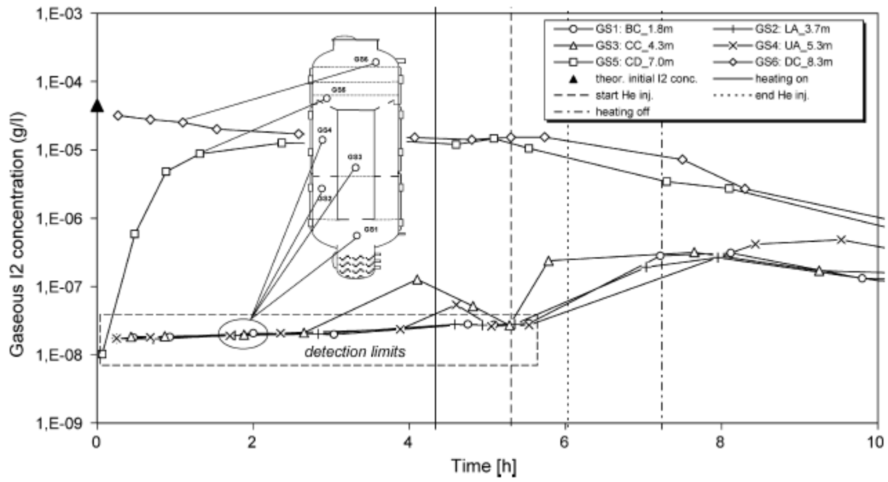


Fig. 2-14 Measured I_2-concentrations in the gas phase of the multi-compartment test Iod-11

The thermal hydraulic nodalisation of the vessel for Iod-11 comprises 50 zones, 73 atmospheric junctions and 58 thermally conducting structures. The nodalisation allows, among other things, the simulation of counter-current flows in the upper and lower annulus and the identification of stratification phenomena in the dome. For COCOSYS-AIM calculations, a nodalisation which deviates from the thermal hydraulic nodalisation can be used for the iodine problem. Two or several thermal hydraulic zones can be combined to one iodine zone (termed as iodine compartment). On the one hand, the different requirements on accuracy of the sub-models are taken into consideration by this and, on the other hand, the calculation time is reduced.

Fig. 2-15 shows the calculated iodine concentrations in the gas phase. During the stratification phase, the I_2 concentration in the sump compartment is below the detection limit and more than three orders of magnitude smaller than in the dome. For hours, no iodine enters the lower compartments. Only with the heat and helium injections, a major natural convection flow is induced by which iodine is slowly transported from the dome into the lower compartments. These convective flows were strong enough for the inert gas helium to become fully mixed in the whole vessel at a test duration of 8.5 hours. But the convective flows were not strong enough to establish a homogeneous iodine distribution in the whole vessel. Until the end of the test, differences in the local I_2 concentrations up to one order of magnitude remain.

In this post-test calculation, the behaviour of the I_2 in the vessel with large local concentration differences during the stratification phase and partly homogenisation of the concentration during the mixing phase is, on the whole, predicted correctly by COCOSYS-AIM. Quantitatively the I_2 concentrations are well calculated for the stratification phase in the lower compartments. But in the mixing phase the increase of the I_2 concentration is overestimated in the upper as well as in the lower compartments. This deviation results from inaccuracies in the iodine sub-model which describes the I_2 resuspension. It appears that a part of the I_2 deposited on the wall has reacted to a non-volatile iodine species unable to resuspend. This process will be investigated further.

The multi-compartment effects on iodine behaviour measured in the ThAI tests are also to be expected in large LWR containments with complex geometries. Their sufficiently accurate simulation is not only essential for the calculation of the iodine source term from the plant but also, due to the high decay heat of the iodine, for the analysis of thermal hydraulics, hydrogen distribution and aerosol behaviour in the containment.

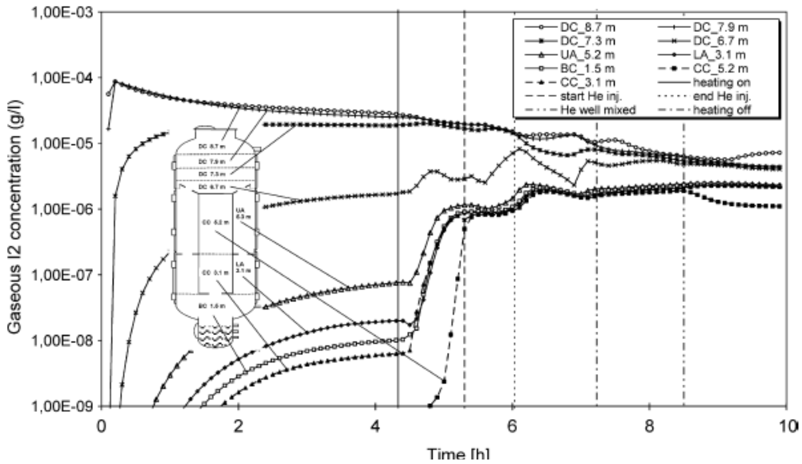


Fig. 2-15 COCOSYS-AIM post-test calculation of the gas phase iodine concentrations in test Iod-11

2.5 COCOSYS Validation by the G02 Bubble Condenser Test

The G02 test was designed to investigate the behaviour of the Bubble Condenser (BC) of NPPs with VVER-440/V-213 in case of a steam line break. The aim of the COCOSYS calculations was to validate the code for these specific conditions /GRS 05/. In October 2002, the G02 test was performed at the facility of the Russian research centre EREC in Elektrogorsk /MEL 03/.

The large-scale BC V-213 test facility (Fig. 2-16) was built at the end of the nineties. It consists of a high-pressure vessel system, hermetic compartments (e. g. steam generator box), an original module of the BC and the so-called air trap. The test facility was scaled 1:100 relative to the containment volume of a VVER-440/V-213. Its total volume is about 520 m³ including 13 tons of water in the BC module. The BC module consists of two segments with nine full-scale gap-cap units each. The test facility is equipped with about 250 gauges to measure temperatures, pressures, differential pressures, mass flow rates, levels, humidity and relief valve opening angle.

The dataset for the post-test calculations with COCOSYS was developed in co-operation with the experts of EREC. It comprises 23 nodes, 34 atmospheric junctions, 21 drainage junctions and 109 heat conduction structures. The initial conditions were chosen in accordance with the values measured before the test. The mass and energy release rate was calculated with the GRS code ATHLET using the values measured for the high-pressure vessel system.

The validation analyses concentrated on pressures and temperatures in the compartment system, pressure difference across the

BC walls and water temperature in the BC. A sensitivity study on the influence of initial and boundary conditions was performed.

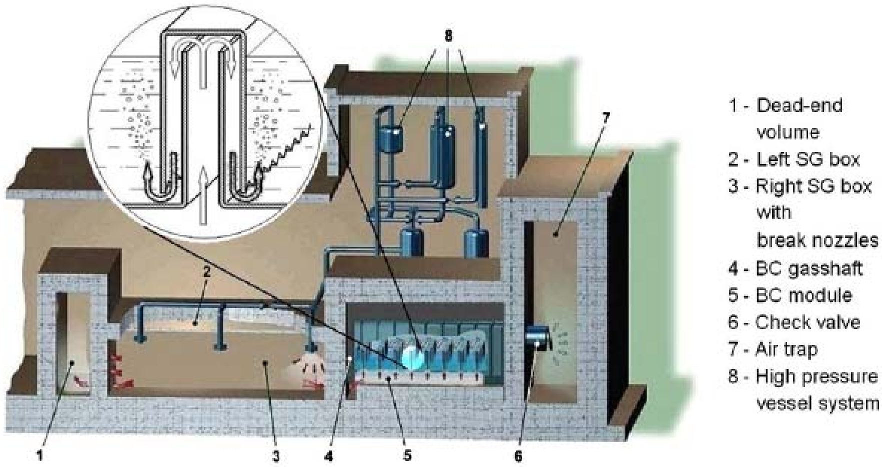


Fig. 2-16 EREC Bubble Condenser Test Facility BC V-213

With regard to pressures (Fig. 2-17) and pressure differences (Fig. 2-18), the validation results show good agreement between measurement and post-test calculations. The grey areas in the figures mark the measurement accuracy of the gauges. A deviating behaviour was calculated for the temperature in the break node. For the total time interval analysed, the calculated temperature is in the superheated range, whereas the measured temperatures were close to saturation. However, one of the three relevant gauges shows some temperature peaks which are an indication to superheated atmospheric conditions. The increase of the water temperature in the BC module provides information about the effectiveness of the BC as pressure suppression system. If this temperature distribution is calculated correctly, an essential objective of the code validation is reached. The COCOSYS results show a good agreement of the calculated water temperature with the arithmetic average of the temperatures measured with the 53 gauges in the water of the BC module (Fig. 2-19).

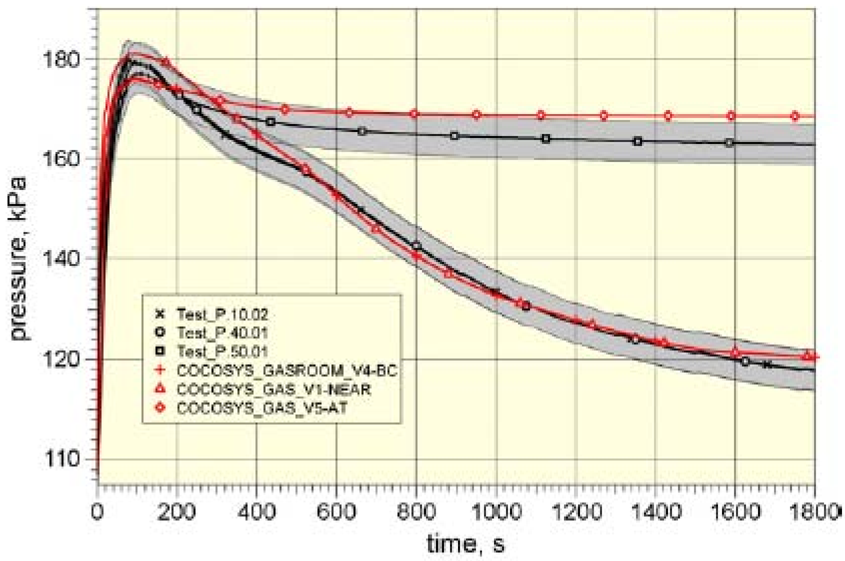


Fig. 2-17 Pressure in right SG box, BC module and air trap

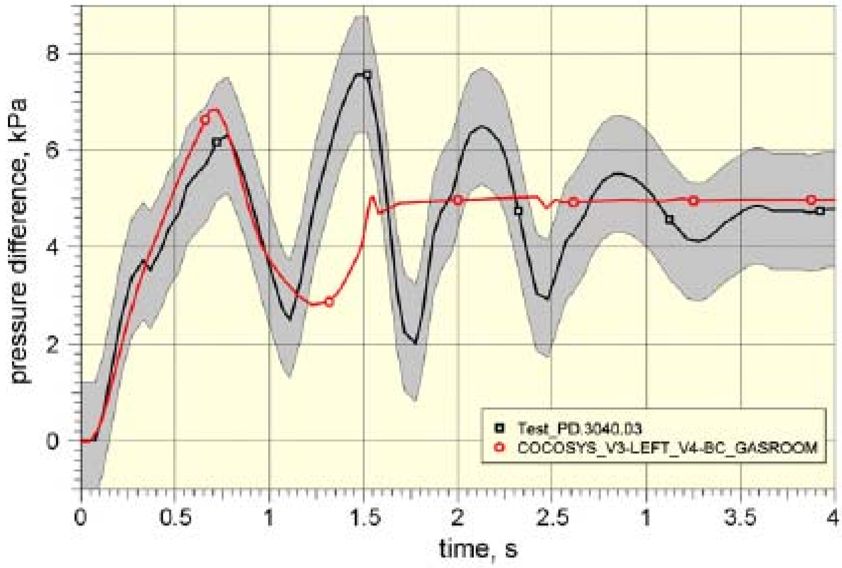


Fig. 2-18 Pressure difference across the BC walls (short term range)

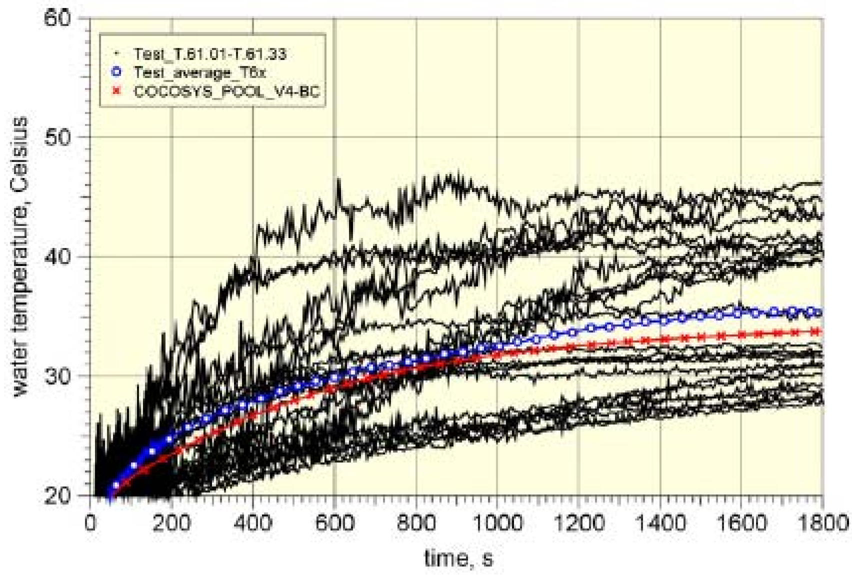


Fig. 2-19 Water temperature in the right section of the BC module

2.6 Validation of Pyrolysis Model on HDR E41.7 Experiment

The implemented pyrolysis model has been tested on the HDR E41-7 Experiment /MAX 94/. The oil experiment has been performed in the burning room 1502, where two doors have been implemented, which could be opened and closed during the experiment. Additionally the burning room could be supplied with fresh air via the HDR inlet ventilation system and from the room 1511. Via three different outlet ventilation systems the hot burned gases could be removed and cleaned by filters. Under this experimental condition forced ventilated conditions with air reversal rates about 5 to 30 as well as natural ventilated and mixed ventilated conditions could be realised. Inside the burning room a $2m^2$ steel pan filled with 40 l of oil was ignited.

For the simulation of the experiment a detailed nodalisation for the complete system has been used. The complete HDR containment has been subdivided into 211 zones (control volumes) connected by 456 junctions. For the simulation of heat transfer into the walls 371 structures have been defined. To consider the local conditions in the fire room it has been subdivided into 4 layers in the main burning part and into 3 layers in the floor part. Each layer consists of 22 zones (Fig. 2-20 and Fig. 2-21).

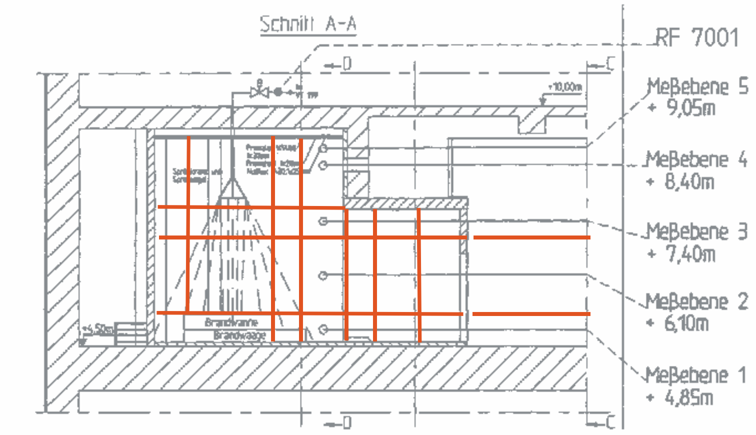


Fig. 2-20 Side view of the fire room

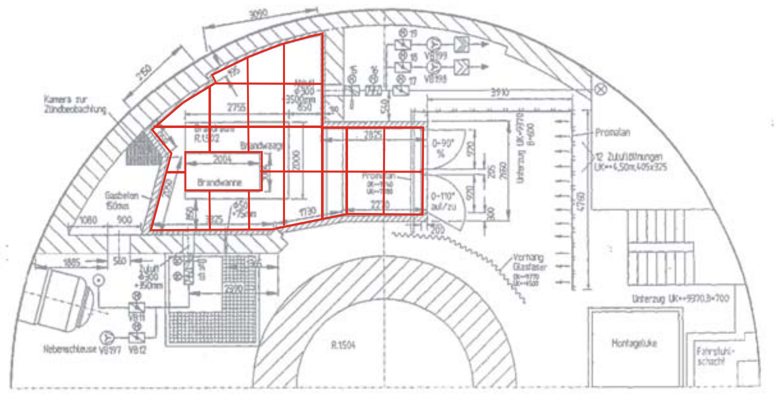


Fig. 2-21 Top view of the fire room

With this nodalisation the stratification in the fire room and the counter current flow through the open doors can be calculated. The floor consists of 3 layers and 4 zones per layer. To avoid artificial convective flow all compartments in the 1500 level have been subdivided into 3 layers too. The rest of the nodalisation of the HDR containment corresponds to that used for the simulation of the HDR E11.4 experiment /SCW 96/.

Fig. 2-22 shows the temperatures inside the fire room at different positions. In comparison to the experiments the calculated temperatures are calculated somewhat to high. The concentrations are calculated quite reasonable (Fig. 2-23). The variations are resulting from the changing of the boundary conditions (ventilation, door position). Fig. 2-24 shows the comparison between the calculated and measured oil mass inside the pan. Fig. 2-25 presents the capabilities of the visualisation tool ATLAS to visualize the dynamic behaviour of the considered system.

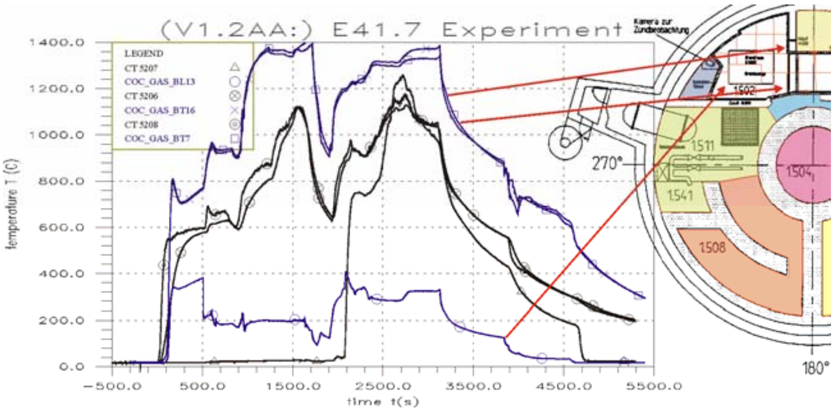


Fig. 2-22 Temperature at different positions in the burning room

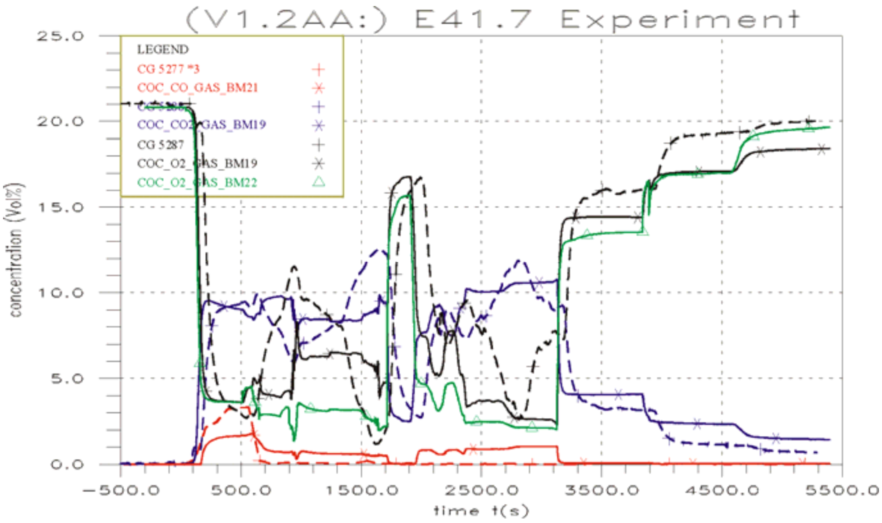


Fig. 2-23 Gas concentrations in the fire room

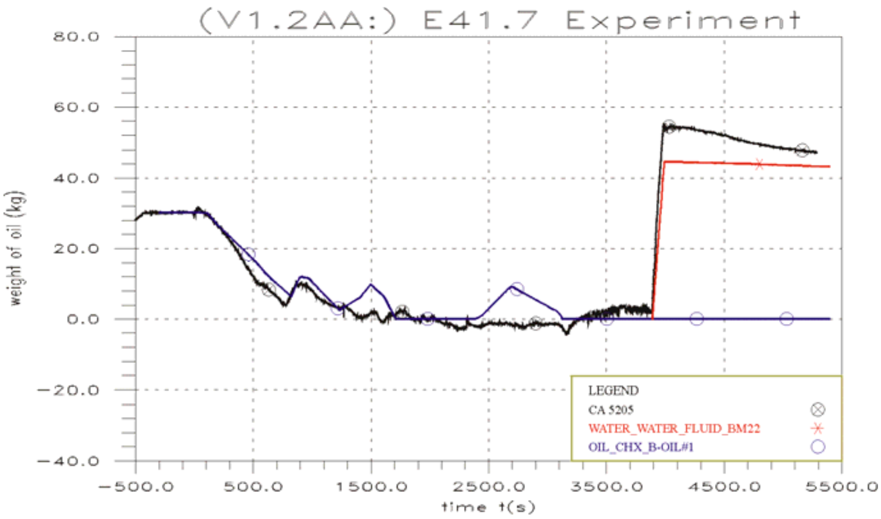


Fig. 2-24 Mass of oil (and spray water)

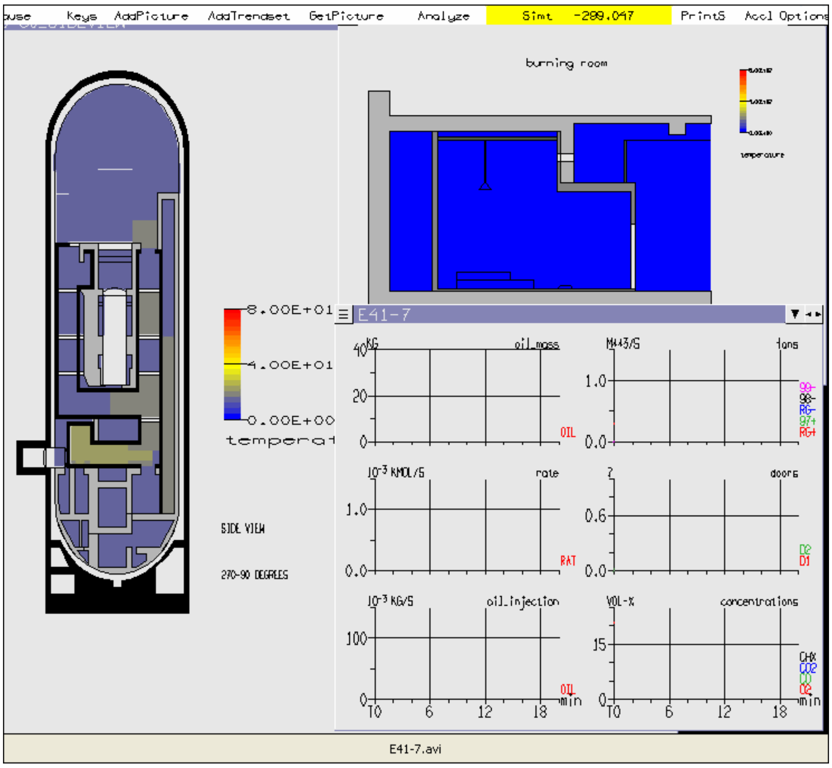


Fig. 2-25 Visualisation of the results

3 Application Examples

3.1 Investigations for the Implementation of Catalytic Recombiners in German PWR's

A large amount of hydrogen is expected to be released within a large dry containment of a PWR shortly after the onset of a severe accident, leading to core degradation and melting. According to local hydrogen accumulation, gas mixture composition, turbulence and structural configuration within the containment, the gas mixture can reach the conditions for deflagration type of combustion or local detonations. As the containment acts as the last barrier against fission product release, careful planned measures are required to prevent hydrogen concentrations reaching a potential level to threat its integrity. Extensive efforts have been given in the past years, to investigate the use of catalytic recombiners to limit the hydrogen concentration in the containment atmosphere during the course of a severe accident. Based on the outcome of these research efforts in Germany it was recommended by the Reactor Safety Commission (RSK) in 1994 to implement catalytic recombiners in large dry containments of PWR plants.

COCOSYS contains a detailed one-dimensional model for the simulation of catalytic recombiners (Fig. 1-6).

A set of representative severe accident scenarios was calculated with the COCOSYS code (see example on Fig. 3-1) taken into account boundary conditions from pre-calculated MELCOR results. Following scenarios have been regarded:

- large break LOCA of surge line (hot leg side),
- small break LOCA of 50 cm^2 on hot leg side, without secondary side cool down,
- station black out with reflooding of the partially destroyed core,
- failure of feed water pumps followed by a primary depressurization.

The installation of catalytic recombiners is a very effective measure to reduce the level of hydrogen in a containment during the propagation of a severe accident but due to specific local conditions the generation of a combustible gas-mixture could not be prevented by the only use of catalytic recombiners. Concerning the distribution following recommendations have been estimated:

- close the main convection paths (e. g. to steam generators),
- inside stair cases in lower, middle and upper position,
- inside so-called dead-end compartments, where a steam-air-hydrogen mixture can enter and with a high potential of steam condensation due to relative low temperatures inside,
- the hot gas plume should not get in contact with safety relevant components.

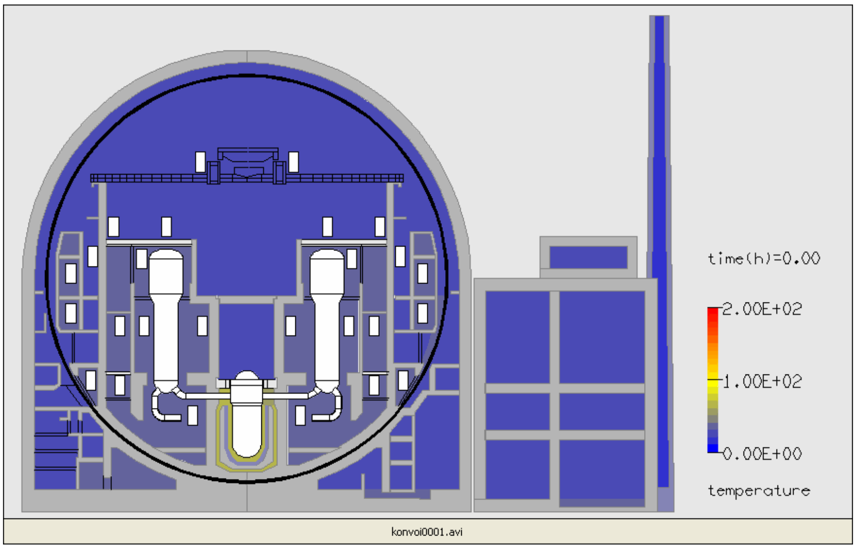


Fig. 3-1 Visualisation of hydrogen distribution and recombination rate

3.2 COCOSYS Application for Russian Designed NPPs

In parallel to the COCOSYS development and validation the code is adapted and applied also to Russian designed NPPs. This work is sponsored by the German government to have a tool answering safety relevant questions for these types of NPPs. Thus, the code was adapted and is applied for all 3 generations of VVER plants as

- VVER-440/V-230 with the original safety relief valves or upgraded by a Jet Vortex Condenser or Circulation Bubble Condenser,
- VVER-440/V-213 with Bubble Condenser (BC),
- VVER-1000/V-320 with large dry containment

and for all generations of RBMK plants as

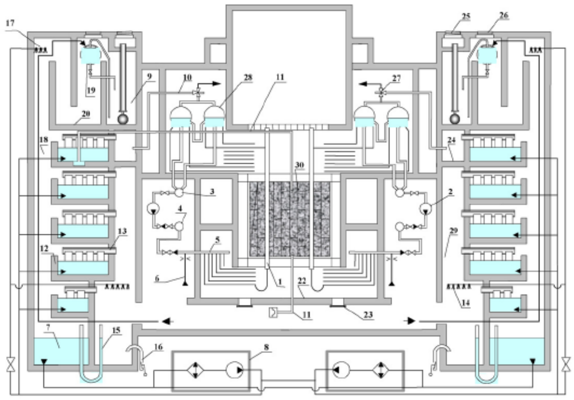
- RBMK-1000 without pressure suppression system (PSS),
- RBMK-1000 with two-floor PSS,
- RBMK-1000 with one-floor PSS,
- RBMK-1500 with PSS located in two accident localization towers with 5 floors each.

To a certain extent the THY main module of COCOSYS was validated for special thermal hydraulic problems of these NPPs.

The COCOSYS code is applied by GRS and by external users in the frame of bilateral and EU projects for VVER and RBMK plants. In the past main focus was paid to thermal hydraulic questions, whereas in the last time the hydrogen distribution and the aerosol and fission product behaviour in case of BDBA and severe accidents get more important.

Recently, an analysis of hydrogen distribution in the accident localisation system compartments of the Ignalina NPP Unit 2 (RBMK-1500, Fig. 3-2) in case of the BDBA scenario "MCP pressure header rupture combined with the total failure of ECCS" was performed. According to the calculation results the design pressures are not reached for any compartment during the whole accident sequence. Most of the hydrogen is concentrated in the BSRC compartments before the condensing pools. The operation of spray systems in these compartments is important because it could lead to a loss of steam inertisation and result in flammable or detonable atmosphere mixtures.

The Kozloduy-3/4 NPP is of VVER-440/V-230 type and the accident localisation system (ALS) was upgraded with a Jet Vortex Condenser and a hydrogen removal and filtered venting system. A parameter study with COCOSYS was performed to investigate the response of the upgraded ALS to a given severe accident scenario with LOCA DN200. The analysis was directed to counter-calculate results of a Bulgarian MELCOR calculation and served to clarify some of the questions identified in the review by GRS. The applied COCOSYS nodalisation (Fig. 3-3) was close to the MELCOR model and also the boundary conditions as mass and energy release rates including hydrogen and decay heat were taken over form MELCOR. The general behaviour of the ALS is to a large extent comparable to the one calculated with MELCOR. Exemplarily, Fig. 3-4 shows the comparison of calculated hydrogen concentrations in the steam generator box. First hydrogen concentration peak at about 0.5 h is caused by the zirconium oxidation during the in-vessel phase and the second after 10 h by the MCCI after RPV failure. The investigation showed that the installations of the filtered venting system and of recombiners are effective severe accident measures, but identified also a need for further approval.



- break location

1 - fuel channel
2 - main circulation pumps
3 - MCP suction header
4 - MCP pressure header
5 - group distribution header
6 - ECCS headers
7 - hot condensate chamber
8 - CTCS pumps and heat exchangers
9 - section of air release pipes
10 - steam pipe from MSV and BRU-B
11 - steam-gas mixture from reactor cavity
12 - condensing pools
13 - steam distribution headers
14 - CTCS sprays in BSRC
15 - water seals/S-traps between HCC and BSRC
16 - BSRC vacuum breakers
17 - CTCS sprays in air venting channel
18 - air venting channel
19 - gas delay chamber tank
20 - gas delay chamber
21 - reinforced leak-tight compartments
22 - LWP compartments
23 - steam discharge valves from LWP to reinforced leak-tight compartments
24 - top steam reception chamber
25 - tip-up hatches
26 - knock-down hatches
27 - MSV and BRU-B
28 - drum separators
29 - steam distribution corridors
30 - reactor

Fig. 3-2 Ignalina-2 NPP, accident localisation system

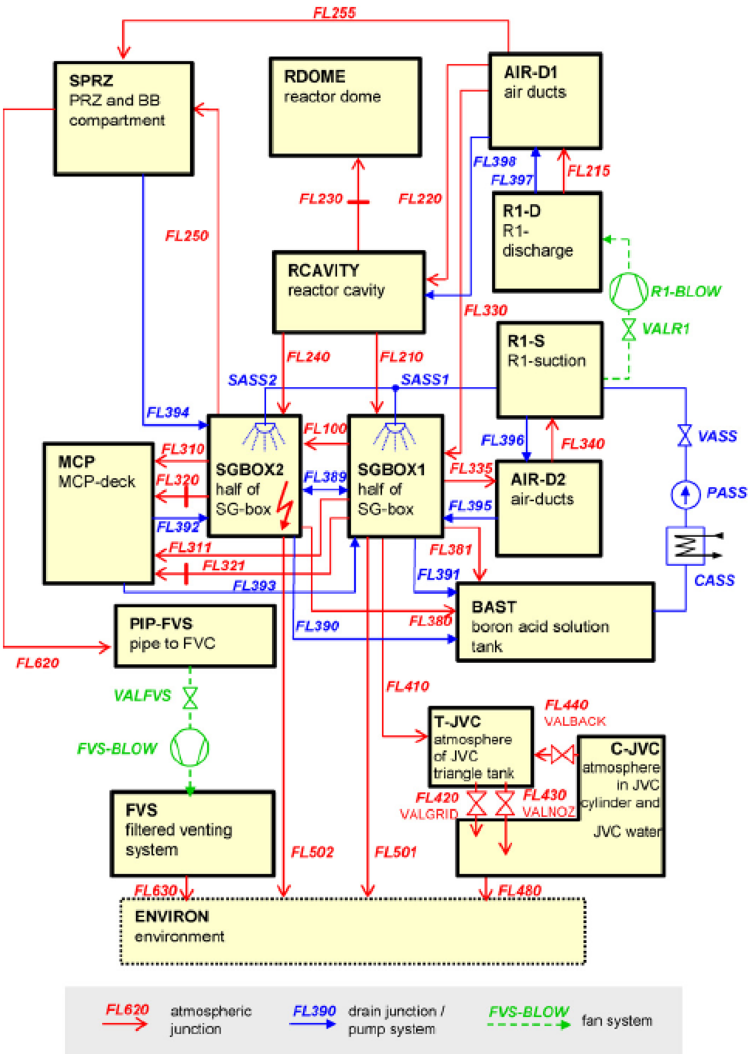


Fig. 3-3 COCOSYS nodalisation, NPP Kozloduy-3/4

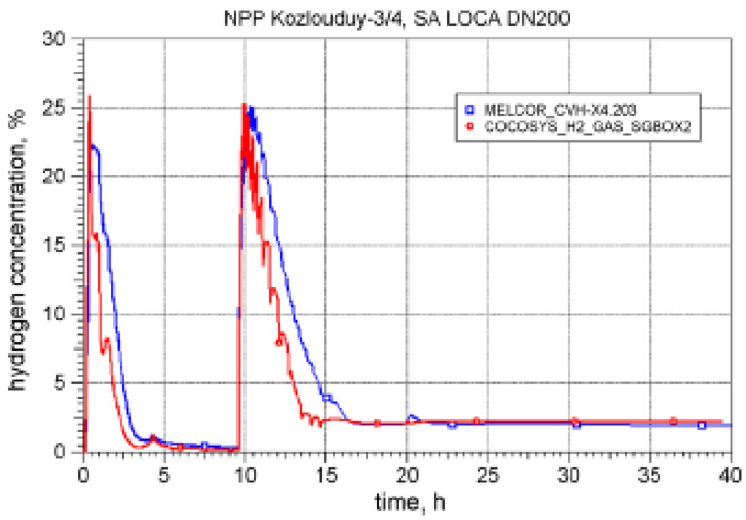


Fig. 3-4 NPP Kozloduy-3/4, SA LOCA DN200, hydrogen concentration in SG box, comparison of COCOSYS and MELCOR results

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