

# ANALYSIS OF THE NODALISATION INFLUENCE ON SIMULATING ATMOSPHERIC STRATIFICATIONS IN THE EXPERIMENT THAI TH13 WITH THE CONTAINMENT CODE SYSTEM COCOSYS

JOERG BURKHARDT\*, SIEGFRIED SCHWARZ<sup>1</sup> and MARCO K. KOCH

Ruhr-Universitaet Bochum (RUB), Energy Systems and Energy Economics (LEE)  
Building IB, 4th Floor, Room 128, Universitaetsstr. 150, 44801 Bochum, Germany

<sup>1</sup> Gesellschaft fuer Anlagen- und Reaktorsicherheit (GRS) mbH, Abteilung Barrierwirksamkeit  
85748 Garching b. Muenchen, Germany

\*Corresponding author. E-mail : Burkhardt@lee.rub.de

*Received January 12, 2009*

*Accepted May 15, 2009*

---

The activities related to this paper are to investigate the influence of nodalisation on simulating atmospheric stratification in the THAI experiment TH13 (ISP-47) with the German containment code COCOSYS.

This article focuses on different nodalisations of the vessel dome, where an atmospheric stratification occurred due to a high helium content. The volume of the dome was divided into several levels that were varied horizontally into different geometries. These geometries differ in the number of zones as well as in the existence of zones that enable the direct rise of an ascending steam plume into the vessel dome. Additionally, the vertical subdivision of the vessel dome was increased to simulate density gradients in a more detailed way.

It was pointed out that the proper simulation of atmospheric stratifications and their dissolution depends on both a suitable horizontal as well as vertical nodalisation scheme. Besides, the treatment of fog droplets has an influence if their settlement is not simulated correctly. This report gives an overview of the gained experience and provides nodalisation requirements to simulate atmospheric stratifications and their proper dissolution.

---

**KEYWORDS** : Thermal Hydraulics, Hydrogen Distribution, Nodalisation Requirements, Atmospheric Stratification

## 1. INTRODUCTION

Within the course of a hypothetical severe accident in a nuclear power plant, hydrogen ( $H_2$ ) can be generated by oxidation processes in the primary circuit and released into the containment. The release of hydrogen at an elevated position could lead to an atmospheric stratification with higher concentrations in the upper part of the containment. Considering the possibility of hydrogen deflagration, the simulation of  $H_2$  distribution by computer codes is of major importance, because the integrity of the containment could be challenged by certain hydrogen combustion modes. These depend on narrow gas concentration bandwidths.

In order to check the reliability of the computer codes and to develop user guidelines and nodalisation rules the codes have to be validated through experiments. The topic of  $H_2$  distribution was covered in the OECD International Standard Problem 47 (ISP-47) by simulating the experiment TH13 in the THAI facility. In this experiment, helium (He)

as a substitute for hydrogen was injected into the vessel and built up a helium enriched atmosphere in the dome. Due to the low density of helium this light gas cloud was strong enough to resist a rising steam plume from breaking into the dome. During the course of the ISP-47 it was pointed out that the simulation of this atmospheric stratification was a big challenge for the participants [1].

## 2. EXPERIMENT TH13 (ISP-47)

The THAI test facility, operated by Becker Technologies GmbH, Germany, is a steel-made cylindrical vessel with a height of 9.2 m and a diameter of 3.156 m. In the experiment TH13, it included an inner steel cylinder (centrally mounted at a height of 2.1 m, length: 4.1 m, diameter: 1.4 m) as well as four condensate trays that were assembled between the inner cylinder and the vessel wall. Fig. 2 (left side) shows an illustration of the test

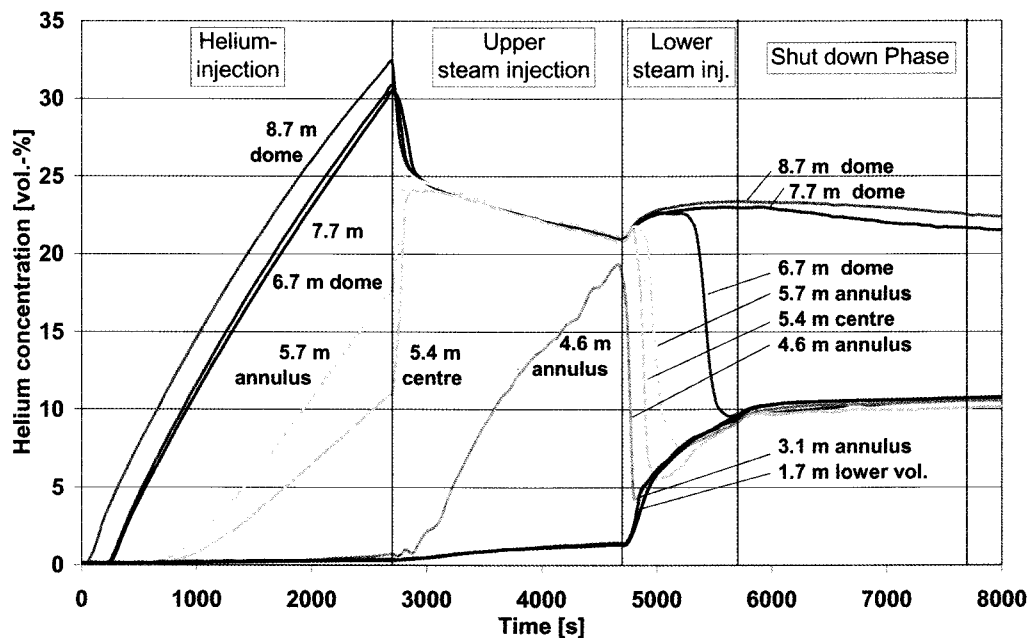


Fig. 1. Measured Helium Concentrations at Different Elevations

vessel. At the beginning of the experiment the atmospheric condition inside the test vessel was the same as in the environment. The procedure of the experiment consists of four phases [1]:

- 0 s – 2.700 s: Upward directed helium injection at a height of 5.8 m (injection velocity = 6.5 m/s, mass flow = 0.6 g/s, pipe diameter = 0.028 m)
- 2.700 s – 4.700 s: Upward directed steam injection at a height of 5.0 m (injection velocity = 24.2 m/s, mass flow = 32.5 g/s, pipe diameter = 0.0443 m)
- 4.700 s – 5.700 s: Horizontally directed steam injection at a height of 1.8 m (injection velocity = 2.7 m/s, mass flow = 35 g/s, pipe diameter = 0.138 m)
- 5.700 s – 7.700 s: Shut down phase, no injection.

Due to the upward directed injection and the low density of the helium, a helium-rich cloud (up to 30 vol.-%) forms in the vessel dome (see Fig. 1, increase of the concentrations in the dome). With a delay of 600 s, the concentrations below the injection (5.7 m and 5.4 m) begin to rise, indicating that helium is pushed downwards into the middle of the vessel. The strong differences in the concentrations between the upper and lower parts of the facility at the end of test phase 1 show atmospheric stratification.

The steam, injected in the 2<sup>nd</sup> phase, also flows into the dome. It mixes with the helium and the air, and pushes the transition layer between the high and low concentrations even further into the middle of the vessel, resulting in a rise of the He concentration at 4.6 m (see Fig. 1).

The horizontally directed steam injection of the 3<sup>rd</sup> phase initiates a plume that mainly rises inside the inner cylinder and causes a subsequent decrease of the

concentrations in the middle of the vessel and the lower part of the dome (see Fig. 1, concentrations at 4.6 m, 5.4 m, 5.7 m, and 6.7 m). It initiates a natural convection that is rising in the inner cylinder and descending in the annulus. This convection mixes the whole vessel atmosphere homogeneously up to a height of 6.7 m. This is demonstrated by the nearly identical concentrations below the height of 6.7 m at the end of phase three.

At the end of the experiment, the concentrations in the dome (at 7.7 m and 8.7 m) remain 12 vol.-% above the ones in the rest of the vessel. The stratification is defending the plume from breaking through [1,2].

### 3. COCOSYS NODALISATION

The program COCOSYS is being developed by the Gesellschaft fuer Anlagen- und Reaktorsicherheit mbH (GRS), Germany, for the simulation of all relevant processes and plant states during severe accidents in containments of light water reactors. COCOSYS is a lumped parameter code.

The input data used as a basis for the simulations was created at RUB-LEE for participation at the ISP-47. It consists of 13 levels with 75 zones that are connected with junctions to enable atmospheric flows. The walls and isolations of the vessel were simulated as heat conducting structures [3].

To analyze the influence of the nodalisation on simulating atmospheric stratifications, the nodalisation of the vessel dome (this is where the helium enriched atmosphere occurred) was varied in different ways. The investigations

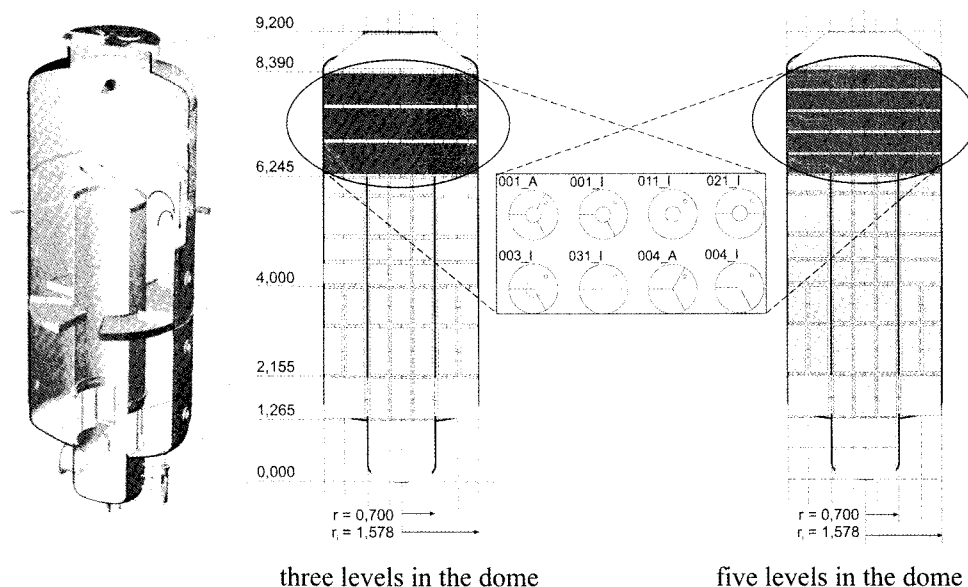


Fig. 2. THAI Vessel, Nodalisation in COCOSYS and Variation of the Vessel Dome

can be divided into the following three steps:

1. The levels (initially three) in the vessel dome were varied horizontally into eight different geometries (see Fig. 2, left nodalisation). These geometries differ in the number of zones as well as in the existence of central zones (see Fig. 2, 001\_A, 001\_I, 011\_I, and 021\_I). These central zones enable the direct rise of the steam plume which ascends in the inner cylinder during the third phase. As a consequence, they have the same diameter as the inner cylinder. In the nodalisations without those zones (see Fig. 2, 003\_I, 031\_I, 004\_A, and 004\_I), the atmosphere flowing out of the inner cylinder is distributed over the whole level above the inner cylinder. This level has a volume five times higher than the volumes of the central zones. Only nodalisation 003\_I has a central zone in the first layer above the inner cylinder. It is a mixture of nodalisations 001\_I and 004\_I and relates to a similar nodalisation that was used by the GRS in the ISP-47 [1].
2. In the second step, the amount of levels in the vessel dome was increased to simulate the vertical density gradients in a more detailed way (see Fig. 2, nodalisation on the right side). These five dome levels were subdivided into the same eight radial nodalisations as in step 1.
3. Based on the results of these investigations, an even finer vertical nodalisation was built with twice the amount of layers in the dome (10 layers, see Fig. 5). In this step, only one radial nodalisation (011\_I) was investigated.

The small dots in the horizontal nodalisation schemes in Fig. 2 symbolize small zones that have been used for simulating the helium plume in the 1<sup>st</sup> phase.

Previous investigations pointed out that the proper

simulation of fog droplets influences the correct simulation of atmospheric densities [5]. The steam injection directed into the dome in the second phase causes the formation of fog droplets [1]. If the sedimentation of these droplets is not simulated, the calculated fog concentration in the dome becomes 5 times higher (ca.  $0.1 \text{ kg/m}^3$ ) than when it was measured in the experiment (about  $0.02 \text{ kg/m}^3$ ). This causes an overestimated atmospheric density in the dome (by ca. 3-4%); therefore, the stratification is dissolved too fast in the third phase. All simulations shown or mentioned in this paper were carried out with a simplified sedimentation model that approximates the fog concentrations quite well (about  $0.012 \text{ kg/m}^3$  in phase 2) [5].

## 4. RESULTS

Fig. 3 shows the results of the simulated helium concentrations (colored thin lines) in the upper and the lower parts of the vessel that were calculated with three layers in the dome. The corresponding measured concentrations (thick black lines) are also included. It can be seen that the first two phases are simulated well by all nodalisations. With the beginning of the third phase, huge differences show up between the radial nodalisations with and without central zones. For this reason their results are described separately in the following sections.

### 4.1 Nodalizations with Central Zones

After a short increase at the start of the 3<sup>rd</sup> phase (4.700 s), which is related to the condensation of steam (see Fig. 3), the calculated concentrations at 8.7 m decrease strongly due to the erosion of the helium-rich cloud caused by the

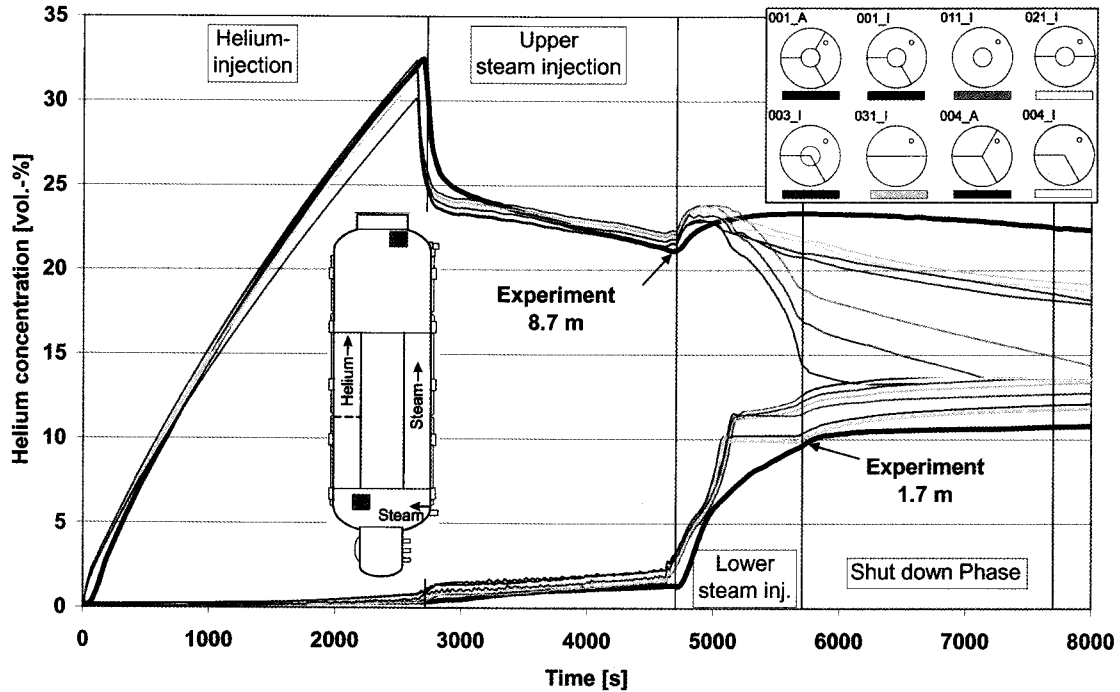


Fig. 3. Simulated and Measured Helium Concentrations, Three Levels in the Dome

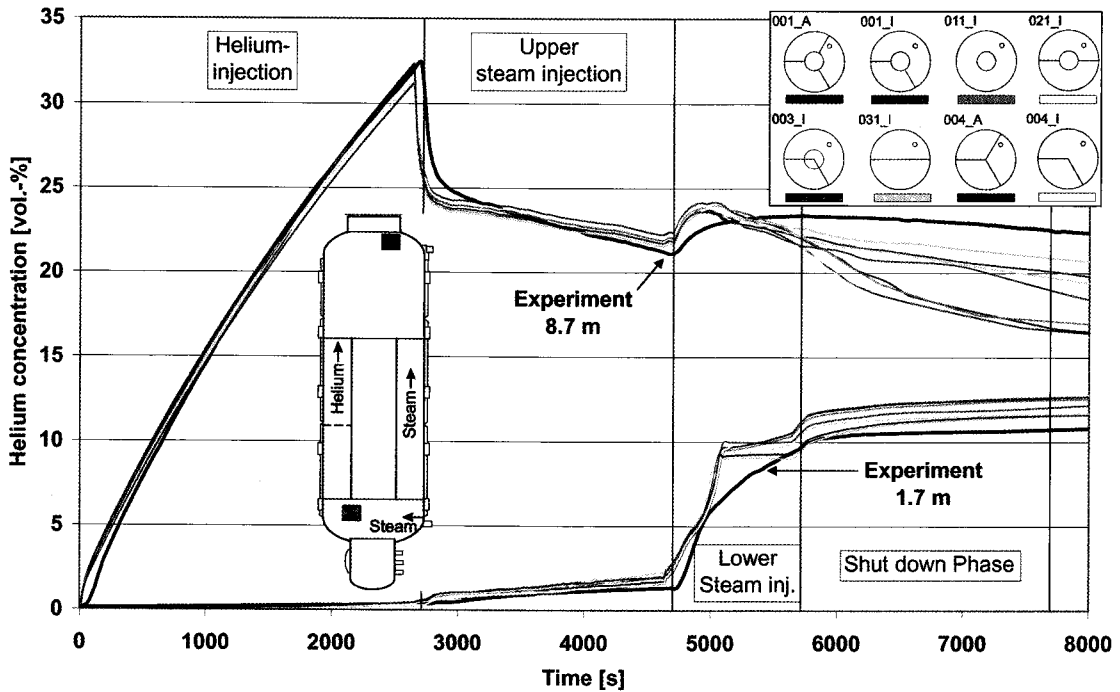


Fig. 4. Simulated and Measured Helium Concentrations, Five Levels in the Dome

ascending plume. In phase four, the concentrations decrease more moderately with nearly half of the speed related to phase three. As a consequence of the strongly decreasing

concentrations, a homogeneously mixed atmosphere is calculated in the whole vessel (the concentrations in the upper and lower parts of the vessel reach the same value)

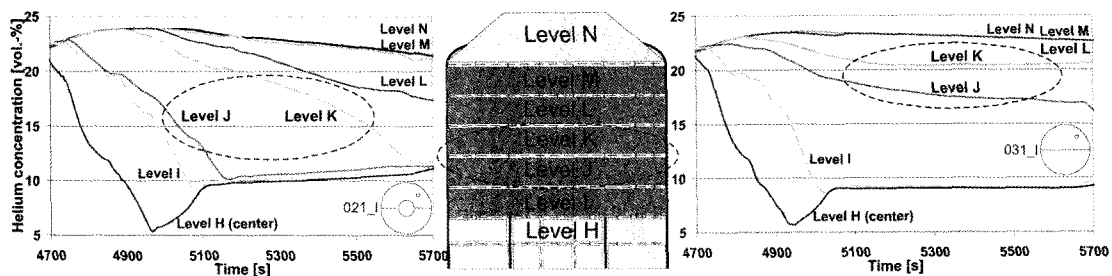


Fig. 5. Comparison of the Simulated Helium Concentrations in the Domes of 021\_I and 031\_I During the 3<sup>rd</sup> Phase, 5 Levels in the Dome

at the end of the experiment. The simulated stratification is not strong enough to defend the rising plume from dissolving the helium-rich cloud in the dome.

This changes with a growing amount of levels in the dome, as can be seen in Fig. 4. The concentrations decrease much slower in the 3<sup>rd</sup> phase and even more moderately in the 4<sup>th</sup> phase. As a result, the ascending plume is not able to dissolve the helium-rich gas cloud in the dome until the end of the experiment. Even if the differences between the concentrations in the dome and the rest of the vessel are simulated to be only 5 vol.-% instead of 12 vol.-% (as it was measured in the experiment), two major facts have to be pointed out:

- The finer vertical nodalisation causes a slower decrease of the concentrations in the 3<sup>rd</sup> and 4<sup>th</sup> phases and makes the simulation of the stratification possible.
- The differences between the diverse radial nodalisations become smaller since nearly the same concentrations are calculated for all of them.

The first point leads to the conclusion that the stratification is calculated to be dissolved more slowly with a finer vertical nodalisation. The results of further investigations concerning this topic are shown in section 4.4.

#### 4.2 Nodalizations without Central Zones

For the nodalisations without central zones, a constant decrease of the concentrations at 8.7 m in phases three and four is calculated (see Figs. 3 and 4). Even though the concentrations are simulated lower than the measured ones, COCOSYS calculates a 6-9 vol.-% higher helium concentration in the dome than in the lower part of the vessel at the end of the experiment. The stable stratification is simulated with three as well as with five levels in the dome.

#### 4.3 Comparison of the Results with and without Central Zones

Comparing the helium concentrations at the top of the facility, the simulation without central zones appears to be more favorable. This is achieved because the atmosphere flowing out of the inner cylinder is distributed over the whole level above the inner cylinder. However, in the experiment, this atmospheric flow forms a buoyant plume

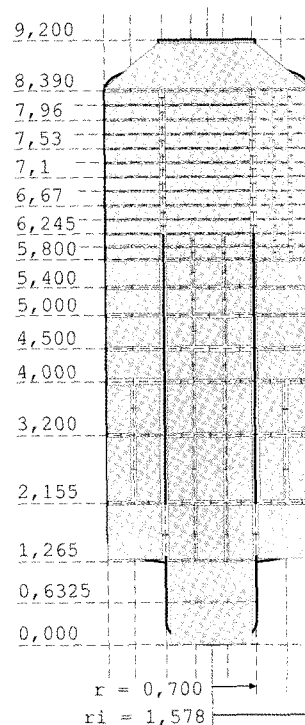


Fig. 6. THAI Nodalisation, 10 Levels in the Dome

which penetrates into the light gas cloud above, dissolving it from the bottom. This is simulated by modeling the central zones: A small buoyancy driven flow rises from the central zone, which is filled with atmosphere coming from the inner cylinder, into the overlying central zone that is still filled with light gas. The density of this overlying zone is therefore increasing gradually. A corresponding small horizontal flow out of this zone also increases the density of the surrounding zones at the “light gas” level with some delay. This results in the approximation of the subsequent drop of the helium concentrations, see Fig. 5 (results for nodalisation 021\_I on the left side, concentrations of level J and level K).

The cases without central zones do not show the

subsequent drop as can be seen in Fig. 5 (results for nodalisation 031\_I on the right side). The concentrations of level J and level K do not fall to the same value as the one in the rest of the vessel but decrease slowly or stay constant until the end of the 3<sup>rd</sup> phase.

As already pointed out in 4.1, the results for the different radial nodalisations with central zones converge with a rising number of levels. Therefore, the results shown in Fig. 5 are representative for all nodalisations of that kind (001\_A, 001\_I, 011\_I, 021\_I).

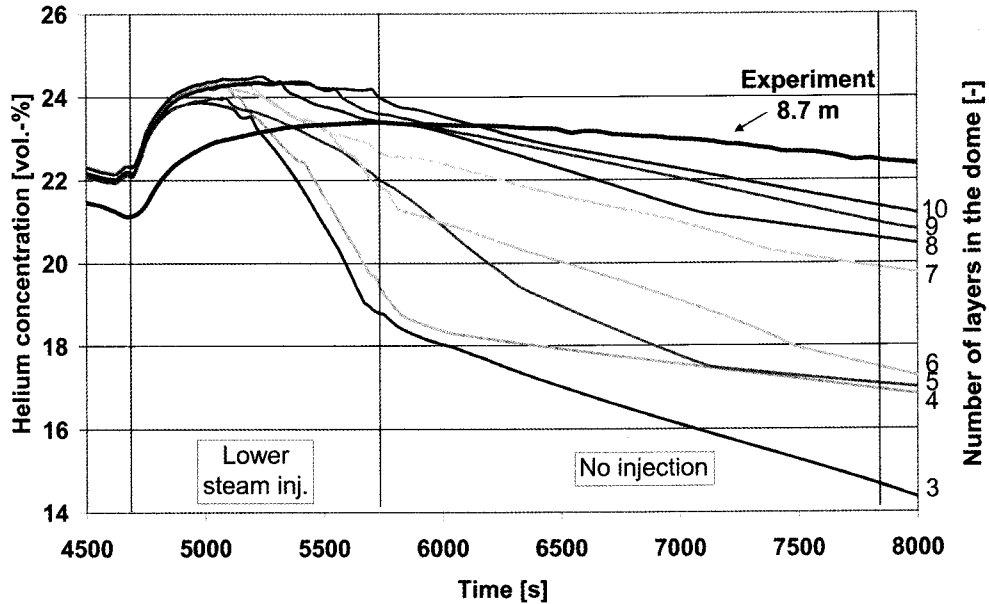


Fig. 7. Measured and Simulated Helium Concentrations with a Varied Amount of Levels in the Dome, 011\_I

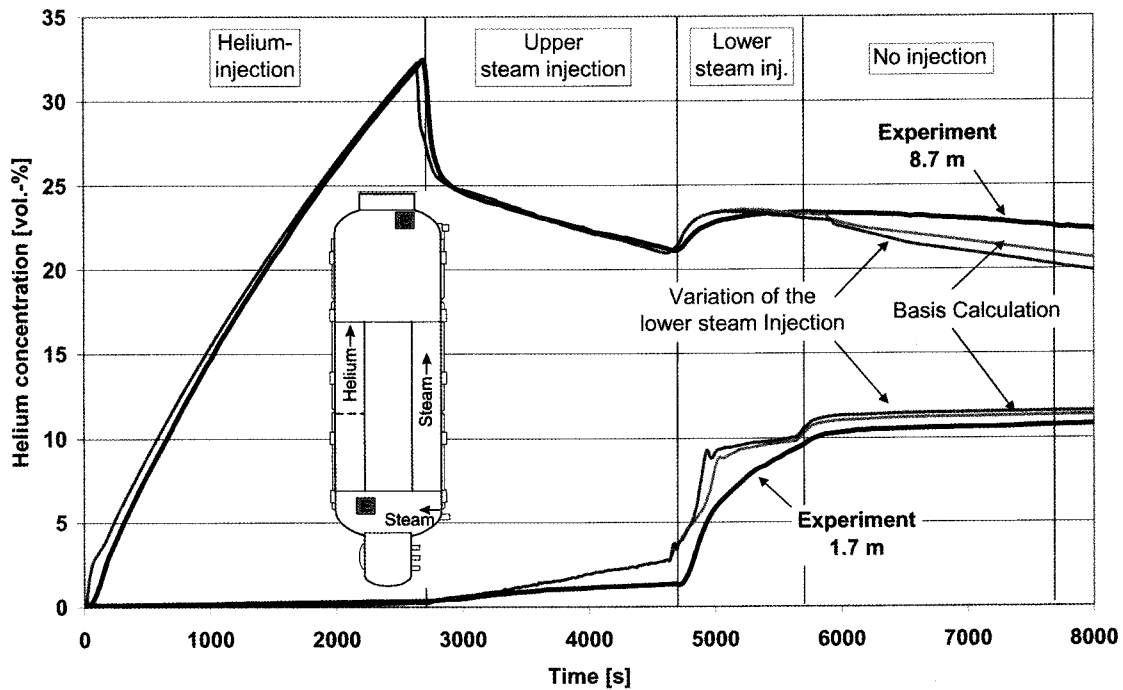


Fig. 8. Simulated and Measured Helium Concentrations, 011\_I, 10 Levels in the Dome

#### 4.4 Further Investigations Concerning the Vertical Nodalisation

To investigate the assumption that the strength of the simulated stratification rises, the finer the vertical nodalisation of the dome gets, its five layers (see Fig. 2, right nodalisation) were divided into ten equally big layers (see Fig. 6).

Due to the fact that the results for all radial nodalisations converge up to equality with a growing number of layers (see Fig. 4), only one, the simplest radial nodalisation (011\_I, see Fig. 2), was taken for these investigations. Another reason is that the THAI vessel only has a diameter of 3.156 m. Only small differences between the thermodynamic values at one height have to be expected in the dome (except between the plume and the surrounding atmosphere). Therefore a complex radial nodalisation does not allow more detailed simulations in here but increases the efforts significantly.

Fig. 7 shows the concentration at 8.7 m for a growing number of layers in the vessel dome. It can easily be seen that the concentration in the dome approaches the experimental value, the finer the vertical nodalisation gets. This also proves that the dissolution process is calculated increasingly correct. Fig. 8 shows the calculated helium concentrations at 8.7 m and 1.7 m, which are calculated well. The concentration at 8.7 m is still decreasing a little bit too fast in the 4<sup>th</sup> phase, but the difference between the concentration in the dome and the rest of the vessel is simulated to be 10 vol.-% (instead of nearly 12 vol.-% in the experiment). The stratification is simulated well.

As Fig. 6 shows, two layers in the middle of the vessel were additionally divided, compared to Fig. 2. This leads to a more detailed calculation of the helium concentration at 8.7 m in the second phase (see Fig. 8) due to a higher transport of helium into the lower vessel. As a consequence, the concentrations in the middle of the vessel are also simulated closer according to the experiment (not shown here).

Additionally, Fig. 8 shows the results of another calculation with a varied simulation of the lower steam injection in phase 3. In the experiment, the horizontal steam jet became a buoyant plume after a short distance, rising mainly in the inner cylinder and partially in the annulus. However, the percentage of the distributed steam between inner cylinder and annulus was fairly uncertain. In the COCOSYS calculations the distribution was estimated by injecting 75% of the steam into the central zone below the inner cylinder and 25% into the annulus zone at the same level. COCOSYS calculates the amount of steam entering the inner cylinder and the annulus. This ratio changes with time during the simulation. In the variation, the steam was completely injected into the central zone below the inner cylinder. The small differences between the results show that the calculations are only slightly sensitive to this variation.

Nearly the same nodalisation (shown in Fig. 6) was successfully used for the blind OECD calculation of the

THAI HM-2 test [4]. In this experiment the complete dissolution of an atmospheric stratification was investigated.

## 5. CONCLUSION

The simulation of an atmospheric stratification and its dissolution with COCOSYS has been investigated. The results of these investigations can be generalized for other applications and the following user guidelines can be given.

For the simulation of the physical flow behavior and the dissolution process the following requirements have to be fulfilled [5]:

- The expected traces of ascending plumes have to be modeled by specific zones, as for example the central zones above the inner cylinder for TH13 (ISP-47).
- The vertical nodalisation of the containment region in which the light gas is located needs to be fine enough (at least five levels) to calculate proper density gradients.
- The influence of the radial nodalisation (number of zones in a level) decreases with a rise in the number of levels. When no big differences have to be expected between the thermodynamic values at the same elevation, a less complex radial nodalisation should be chosen.

These requirements have also been used in the blind calculation of the experiment THAI HM-2 and are confirmed by the good results [4]. They have also been discussed with and transferred to the GRS and will be included in the upcoming COCOSYS user manual. These user guidelines are also valid for other Lumped Parameter codes; they have been successfully applied to an open simulation of HM-2 with MELCOR [6].

## ACKNOWLEDGMENTS

The work concerning TH13 is sponsored by the German Federal Ministry of Economics and Technology (BMWi) under the contract number 1501321. This work is additionally supported by the Ruhr-Universität Research School funded by the DFG in the framework of the Excellence Initiative [DFG GSC 98/1]. The authors would like to thank Dr. Mohammed Bendiab (RUB-LEE until June 2008) for the valuable discussions.

## REFERENCES

- [ 1 ] H.-J. Allelein, K. Fischer, J. Vendel, J. Malet, E. Studer, S. Schwarz, M. Houkema, H. Paillere, A. Bentaib: "International Standard Problem ISP-47 on Containment Thermohydraulics." Final Report, JT03231730, Nuclear Energy Agency (NEA), France (2007).
- [ 2 ] T. Kanzleiter, G. Ahrens, K. Fischer, W. Häfner, A. Kühnel, G. Poss, F. Funke, G. Langrock, H.-J. Allelein, G. Weber, S. Schwarz, "Versuchsanlage und Programm zur Untersuchung offener Fragen zum Spaltproduktverhalten Im Sicherheitsbehälter, ThAI Phase II, Teil 1." 1501272-S1, Becker Technologies, Eschborn, Germany (2007).
- [ 3 ] M. Bendiab, M. Dapper, H.-J. Wagner, H. Unger, M. K.

- Koch: "Simulation des ThAI-Versuchs (TH13) im Rahmen des ISP-47 mit dem Containment Analysecode COCOSYS." 5th Technical Report of the Project BMWi No. 150 1242, LEE-29, Bochum, Germany (2005).
- [ 4 ] K. Fischer: "Comparison of Experimental Data and Blind Calculations of Test HM-2." Report Nr. 1501326 – HM-2, Becker Technologies GmbH, Eschborn, Germany (2008).
- [ 5 ] J. Burkhardt, M. Dapper, M. Kloecker, H.-J. Wagner, M. K. Koch: "Simulation atmosphärischer Schichtungen in den Versuchen TH12 und TH13 (ISP-47) mit dem Programmsystem COCOSYS." LEE-48, Ruhr-Universität Bochum, Germany (2008).
- [ 6 ] J. Duspiva, "Post Test Calculation of OECD THAI HM-2 Experiment with MELCOR 1.8.6 Code," NURETH-13, Kanazawa, Japan, September 27 - October 2, 2009, N13P1122 (2009).