

LAPPEENRANTA UNIVERSITY OF TECHNOLOGY

Faculty of Technology

LUT Energy

Energy Technology

Jarno Kolehmainen

**MODELLING OF HYDROGEN STRATIFICATION AND GAS
MIXING IN CONTAINMENT USING THE APROS CODE**

Examiners: Professor, D.Sc (Tech) Riitta Kyrki-Rajamäki

Professor, D.Sc (Tech) Juhani Hyvärinen

Supervisors: D.Sc (Tech) Markku Hänninen

M.Sc (Tech) Ari Silde

ABSTRACT

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Jarno Kolehmainen

Modelling of hydrogen stratification and gas mixing in containment using the APROS code

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Hydrogen stratification and atmosphere mixing is a very important phenomenon in nuclear reactor containments when severe accidents are studied and simulated. Hydrogen generation, distribution and accumulation in certain parts of containment may pose a great risk to pressure increase induced by hydrogen combustion, and thus, challenge the integrity of NPP containment. The accurate prediction of hydrogen distribution is important with respect to the safety design of a NPP.

Modelling methods typically used for containment analyses include both lumped parameter and field codes. The lumped parameter method is universally used in the containment codes, because its versatility, flexibility and simplicity. The lumped parameter method allows fast, full-scale simulations, where different containment geometries with relevant engineering safety features can be modelled. Lumped parameter gas stratification and mixing modelling methods are presented and discussed in this master's thesis.

Experimental research is widely used in containment analyses. The HM-2 experiment related to hydrogen stratification and mixing conducted at the THAI facility in Germany is calculated with the APROS lump parameter containment package and the APROS 6-equation thermal hydraulic model. The main purpose was to study, whether the convection term included in the momentum conservation equation of the 6-equation modelling gives some remarkable advantages compared to the simplified lumped parameter approach. Finally, a simple containment test case (high steam release to a narrow steam generator room inside a large dry containment) was calculated with both APROS models. In this case, the aim was to determine the extreme containment conditions, where the effect of convection term was supposed to be possibly high. Calculation results showed that both the APROS containment and the 6-equation model could model the hydrogen stratification in the THAI test well, if the vertical nodalisation was dense enough. However, in more complicated cases, the numerical diffusion may distort the results. Calculation of light gas stratification could be probably improved by applying the second order discretisation scheme for the modelling of gas flows. If the gas flows are relatively high, the convection term of the momentum equation is necessary to model the pressure differences between the adjacent nodes reasonably.

TIIVISTELMÄ

Lappeenrannan teknillinen yliopisto
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LUT Energia
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Jarno Kolehmainen

Vedyn kerrostumisen ja kaasujen sekoittumisen mallinnus suojarakennuksessa APROS ohjelmistolla

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Tarkastajat: Professori Riitta Kyrki-Rajamäki, Professori Juhani Hyvärinen

Hakusanat: APROS, suojarakennusmallinnus, lumped parameter -menetelmä, vedyn kerrostuminen, THAI

Ydinvoimalaitosten vakavien onnettomuuksien tutkimuksen yksi tärkeä osa-alue on kaasujen kerrostuminen ja sekoittuminen suojarakennuksessa. Suojarakennuksen eheyden varmistaminen on yksi tärkeimmistä turvallisuustoiminnoista vakavan onnettomuuden kannalta. Vakavan onnettomuuden aikana syntyy runsaasti vetyä ja lauhutumattomia kaasuja, joiden kertyminen suojarakennukseen voi aiheuttaa vetyräjähdysten ja suojarakennuksen paineen nousun kautta eheyden vaarantumisen.

Suojarakennusmallinnuksessa käytettävät yleisimmät laskentamenetelmät ovat lumped parameter -menetelmät sekä kenttäohjelmistot. Useimmissa suojarakennusohjelmissa käytetään lumped parameter -menetelmää sen monipuolisuuden, joustavuuden ja helppokäyttöisyyden takia. Lumped parameter -menetelmä mahdollistaa nopeat täyden mittakaavan simulaatiot erilaisissa suojarakennusgeometrioissa. Tässä työssä keskitytään lumped parameter -menetelmään suojarakennuksen kaasutilan sekoittumisen ja kerrostumisen mallintamisen kannalta.

Vedyn kerrostumisen ja sekoittumisen laskentaa vertailtiin laskemalla THAI koe HM-2 käyttäen APROS lumped parameter suojarakennusohjelmaa sekä APROS kuusiyhtälömallia. Tällä vertailulla haluttiin tutkia vaikuttaako kuusiyhtälömalliin ohjelmoitu liikemäärän välitystermi merkittävästi laskentatuloksiin verrattuna lumped parameter mallin yksinkertaisempaan laskentamalliin. Molemmat laskentamenetelmät laskivat kokeen hyvin kun noodistus on riittävä. Lisäksi molemmilla laskentamalleilla laskettiin yksinkertainen suojarakennuslasku, jossa suuri höyryvuoto purkautuu ahtaaseen tilaan, joka kuvaa suojarakennuksen höyrytilaa. Simulaatioiden perusteella voidaan päätellä että suurten virtausten tapauksissa liikemäärän välitystermin lisääminen laskentaan voisi olla hyödyllistä muodostuvien huoneiden välisten painerojen kannalta. Testi simulaatioiden perusteella numeerinen diffuusio voi vääristää laskentatuloksia monimutkaisissa tapauksissa. Laskenta mallia voisi kehittää lisäämällä toisen kertaluvun diskretoinnin kaasuvirtauksien laskentaan.

PREFACE

This thesis was written in the Nuclear power plant behaviour team at VTT Technical Research Centre of Finland. The supportive atmosphere at VTT helped me greatly during the work.

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ABBREVIATIONS AND SYMBOLS

APROS	<i>Advanced Process Simulation Software</i>
BE	<i>Best Estimate</i>
CFD	<i>Computational Fluid Dynamics</i>
DBA	<i>Design-Basis Accident</i>
DCH	<i>Direct Containment Heating</i>
FCI	<i>Fuel-Coolant Interactions</i>
GRS	<i>Gesellschaft für Anlagen- und Reaktorsicherheit</i>
MCCI	<i>Molten Core-Concrete Interaction</i>
NPP	<i>Nuclear Power Plant</i>
ISP	<i>International Standard Problem</i>
LDA	<i>Laser Doppler Anemometry</i>
LP	<i>Lumped Parameter</i>
LOCA	<i>Loss of Coolant Accident</i>
LWR	<i>Light Water Reactor</i>
OECD	<i>Organization for Economic Cooperation and Development</i>
PAR	<i>Passive Autocatalytic Recombiner</i>
PRA	<i>Probabilistic Risk Assessment</i>
PSA	<i>Probabilistic Safety Assessment</i>
PWR	<i>Pressurised Water Reactor</i>
RPV	<i>Reactor Pressure Vessel</i>
SA	<i>Severe Accident</i>
SBLOCA	<i>Small Break Loss of Coolant Accident</i>
SESAR	<i>Senior Group of Experts on a Nuclear Safety Research</i>
STUK	<i>Radiation and nuclear safety authority</i>
THAI	<i>Thermal-hydraulics, Hydrogen, Aerosols and Iodine</i>

Latin letters:

F	friction force /volume	$\left[\frac{\text{N}}{\text{m}^3} \right]$
g	acceleration of gravity	$\left[\frac{\text{m}}{\text{s}^2} \right]$
h	specific enthalpy	$\left[\frac{\text{J}}{\text{kg}} \right]$

p	pressure	[Pa]
q	heat flow/volume	$\left[\frac{\text{W}}{\text{m}^3}\right]$
S	source term	
t	time	[s]
u	velocity	$\left[\frac{\text{m}}{\text{s}}\right]$
w	velocity of mixture	$\left[\frac{\text{m}}{\text{s}}\right]$

Greek letters:

α	volume fraction of phase	
ρ	density	$\left[\frac{\text{kg}}{\text{m}^3}\right]$
Γ	mass change rate	$\left[\frac{\text{kg}}{\text{m}^3\text{s}}\right]$

Subscripts:

g	gas phase
i	interface of phases
i	mass
j	momentum
k	phase (liquid or gas)
k	energy
nc	non-condensable gas
w	wall of a flow channel
z	space coordinate

Chemical labels:

CO_2	Carbon dioxide
Cr	Chrome
Cr_2O_3	Chromium (III) oxide
H_2	Hydrogen
H_2O	Water
N_2	Nitrogen
O_2	Oxygen

UO_2	Uranium dioxide
Zr	Zirconium
ZrO_2	Zirconium dioxide

1 INTRODUCTION

Nuclear power plant (NPP) containment is the last safety barrier in a series of barriers against a release of fission products to the environment during severe accidents (SA) (Povilaitis et al. 2011, 1). The integrity of the containment must be ensured. Thermal hydraulic processes inside the containment, especially the behaviour of non-condensable gases and steam in a response to a postulated accident, are important issues in respect of NPP safety. (Zboray et Paladino 2010, 1.)

Large amount of hydrogen may be generated in the core degradation process mainly when steam oxidises zirconium in the reactor core. Another potential hydrogen source in a severe accident is a molten core concrete interaction (MCCI) on bottom of the containment system. Consequently, generated hydrogen may be released into the containment. If the hydrogen concentration reaches the flammability limit, ignition is possible and the pressure loads caused by combustion may produce a threat to the containment integrity. (OECD 1999, 6 ; Burkhardt et al 2009, 1.)

The modelling of distribution of the generated hydrogen in containment atmosphere is still an open issue (Studer et al. 2007, 1). The distribution of hydrogen has to be modelled sufficiently accurately to obtain initial conditions of a subsequent combustion process, in order to assess the combustion hazard to the containment system (OECD 2007, 15).

The containment package of Advanced process simulator software (APROS) is one of the many computer codes that can be used in lumped parameter (LP) containment analyses. Traditionally, the LP codes have been mainly used to assess the containment pressure and temperature response in postulated accidents. However, despite certain modelling limitations and simplifications of LP codes, use of the LP approach also in analysing the stratification of gases in the containment atmosphere has been extensively used. Lumped parameter models do not consider momentum convection from one node to another. The traditional trend has been to favour coarse nodalizations in LP codes for accident analyses. In this approach, one node typically corresponds to separate room

with solid walls. However, during the last years this trend has been challenged. Recently a novel modelling concept has been studied and developed, where open volumes of containment atmosphere are divided into several sub-nodes. By dividing the open volume into several sub-nodes it is possible to use LP method to model stratification problems.

The main aim of this master's thesis is to study the LP modelling of hydrogen mixing and stratification in a containment using the APROS containment package. In addition, an influence of the flow convection term of the momentum conservation equation on the stratification modelling is studied. The convection term is included in the 1-D APROS six-equation model, but not in the APROS LP containment package. Therefore, both the APROS containment and six-equation models are used to calculate the THAI experiment HM-2 (hydrogen/helium transport and mixing). The aim of the calculations are to investigate, whether the convection term in the momentum equation of the six-equation model gives some remarkable advantages in modelling of the light gas stratification, compared to the simplified lumped parameter approach. In addition, a simple containment test case (high steam release to a narrow steam generator room inside a large dry containment) was calculated with both APROS models. In this case, the aim was to determine the extreme containment conditions, where the effect of convection term was supposed to be possibly high.

In Chapter 2, a literature study of general safety aspects of NPP containment atmosphere is given. Also the phenomena/methods associated with atmosphere mixing, stratification of hydrogen, hydrogen management and modelling these phenomena in lumped parameter codes are presented. Chapter 3 covers the main calculation methods used in NPP containment analysis and research. Chapter 4 discusses calculation codes used in NPP containment analyses. APROS containment package and the APROS six-equation model are described, because they are used in the computational part of this thesis. In Chapter 5 the THAI test facility and its instrumentation are described. In Chapter 6 the computational results of the APROS containment and the six-equation models are compared to the results of the HM-2 experiment. In addition, the calculation results of the simple test cases are also presented. Chapter 7 presents the conclusions of the comparison of used APROS-models.

2 GENERAL SAFETY ASPECTS OF NUCLEAR POWER PLANT

Safety is a very important aspect to be considered in nuclear energy production. Nuclear safety research contains safety research of the reactors, nuclear fuel, systems and components used in NPP and accident analysis. Nuclear safety has been studied since the concept of a nuclear fission was utilized in energy production. All NPPs must fulfil safety demands and criterions. The important safety functions of light water reactors (LWR) are the reactor shutdown to ensure criticality safety, removal of decay heat from the reactor to the ultimate heat sink and prevention of release of radioactive material by ensuring integrity of the safety barriers of NPP such as fuel cladding, primary coolant system and containment. By nuclear safety research, implementation of safety functions is guaranteed during the whole operation of the NPP. (STUK 2008, 1-7.)

Nuclear accident research concentrates on prevention, mitigation and gaining knowledge of different kinds of hypothetical accidents. Safety research includes safety assessment, use of analytical tools, modelling, calculating and experimental research. One specialised area of the calculation codes is modelling of the thermal hydraulic behaviour of containment atmosphere.

Plant data from accidents is extremely scarce because the accident data cannot be obtained from normally operating NPPs. Full-scale facility experiments are not feasible, so safety research must rely on the small and medium-scale experiments. Experiments have been done in different thermohydraulic facilities to understand the occurring phenomena during postulated accidents. Data extracted from the experiments are compared to the calculation results of the computer codes. The comparison results are used in the validation process of the codes. All the calculation codes used in NPP safety research and analyses must be validated in order to guarantee their sufficient reliability. (Burkhardt et al. 2009, 1.)

2.1 Containment Safety Function

The first barrier against radioactive materials is gas proof cladding of nuclear fuel. The second barrier is primary circuit. The containment is the last safety barrier of NPP that

prevents a release of radioactive materials into the environment in accidents (OECD 1999, 16, 32.). Figure 1 shows the defence-in-depth safety barriers of a nuclear power plant. (STUK 2008, 3-4.) Establishing and maintaining the integrity of the NPP containment during accidents is one of the major topics in nuclear safety research. The containment integrity may be challenged e.g. by overpressurisation due to energetic releases of liquid, steam and non-condensable gases into the containment e.g. in loss-of-coolant accidents (LOCA) or main steam line break accidents and due to combustion of flammable gases (such as hydrogen) during severe accidents. (OECD 1999, 16, 32.) Other events that could cause over pressurization during SA are e.g. MCCI, direct containment heating (DCH), steam explosions and hydrogen-air deflagration (OECD 1999, 22-25.). Severe accidents are defined as accidents, where most of the fuel in reactor core loses its original structure (STUK 2008, 4).

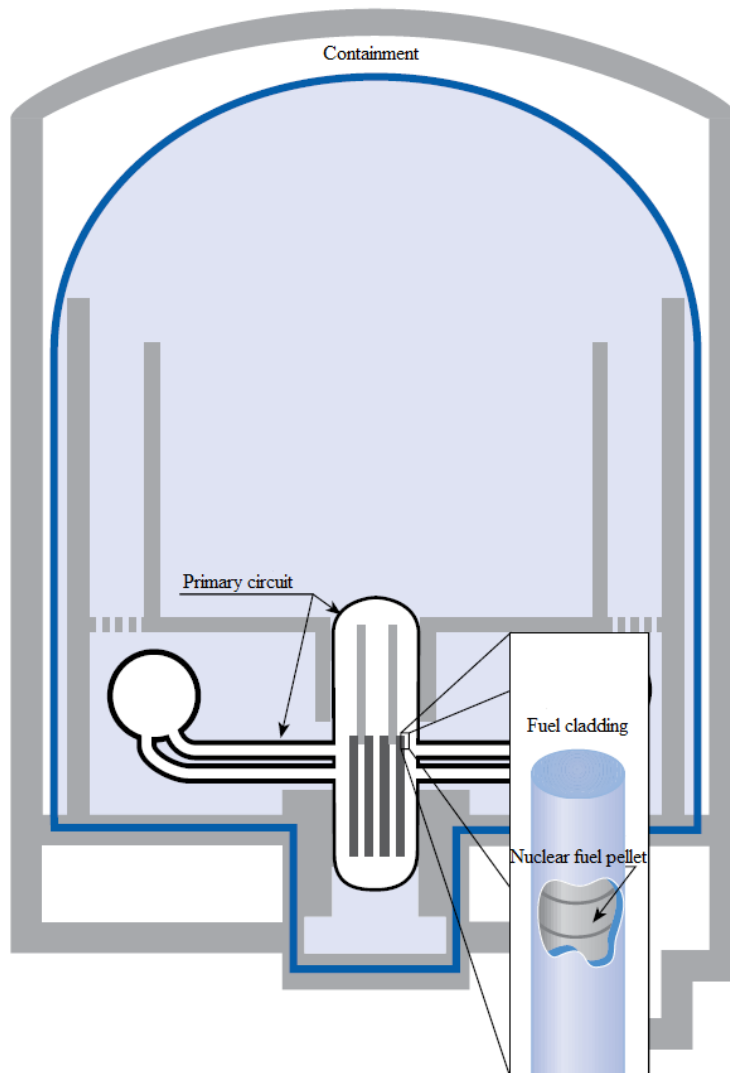


Figure 1. In-depth safety barriers of NPP (STUK 2008, 4)

2.2 Hydrogen in Containment Atmosphere during Severe Accidents

The possibility that hydrogen could be generated as result of an oxidation process in the core, leak to the containment atmosphere and form a stratified volume that could burn and thus jeopardise the integrity of the containment has to be minimised by research, testing and administrative measures. (Burkhardt et al. 2009, 1.) Therefore the ability to predict the hydrogen behaviour in the containment by the computer codes has been a major research topic (Schwarz et al. 2011, 1).

2.2.1 Hydrogen Generation

In severe NPP accidents, hydrogen is generated by exothermic reaction between steam and zirconium, when the temperature in the core rises above 1200°C. (Payot et al. 2012, 2). The maximum amount of generated hydrogen in a severe accident can rise to the order of one metric ton, depending on the reactor design and size (Payot et al. 2012, 2). Hydrogen can be generated also in other means, but the oxidation is the most important process (Valdés-Parada et al. 2013, 1).

Hydrogen generation in the reactor pressure vessel (RPV) during core melt requires high temperature, availability of steam and un-oxidized reaction partners, contact surface and reaction time. The most of the zirconium in the reactor is in the fuel cladding. The dominant oxidation processes for zirconium fuel cladding, structural materials of the reactor core and nuclear fuel are presented in equations 1, 2 and 3 (Kljjenak 2013).



$$\text{with } 0 < x < 0.1$$

There are also some ex-vessel SA phenomena which have a potential to produce hydrogen such as DCH, in which molten core debris disperse in containment, MCCI and molten fuel-coolant interactions (FCI). The “ex-vessel phenomena”, means that they become active after the RPV has failed, and the molten reactor core and internals are relocated. The DCH, FCI and MCCI processes may oxidize large fraction of metals of the core melt. Figure 2 presents the typical hydrogen generation rates from different processes. (Kljjenak 2013.)

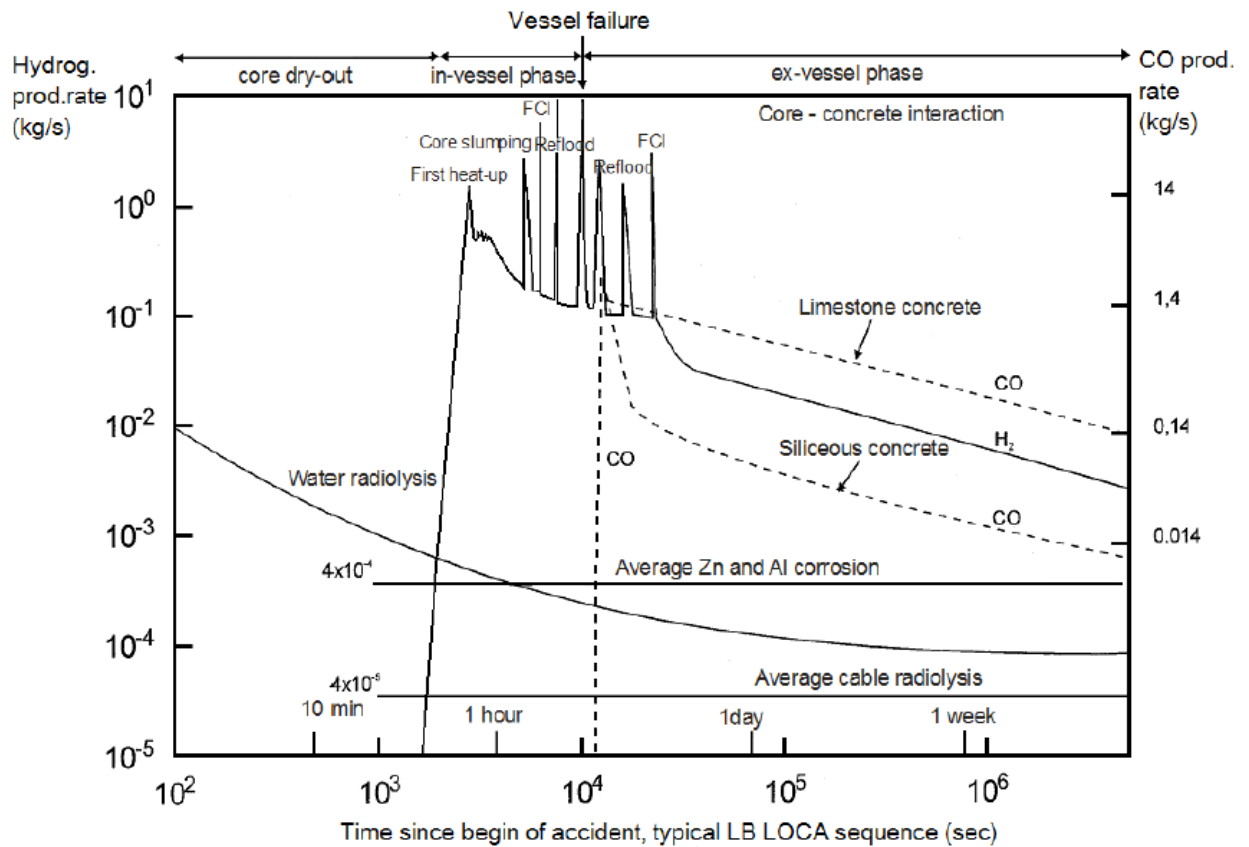


Figure 2. Typical hydrogen generation rates during severe accident (Kljcnak 2013)

Hydrogen can ignite and burn or detonate in certain steam and air concentrations. Flammability limits where different hydrogen combustion modes are possible may be characterised by the combination of concentrations of steam, oxygen (air) and the combustible gas (hydrogen). Only narrow concentration bandwidths define the expected combustion modes. (Mallet et al. 2010, 1.) The most common flammability diagram is the Shapiro diagram (Figure 3). The burn limit in the diagram describes the limits, where the hydrogen deflagration is possible, and the detonation limit in the diagram describes the limits, where the hydrogen detonation is possible.

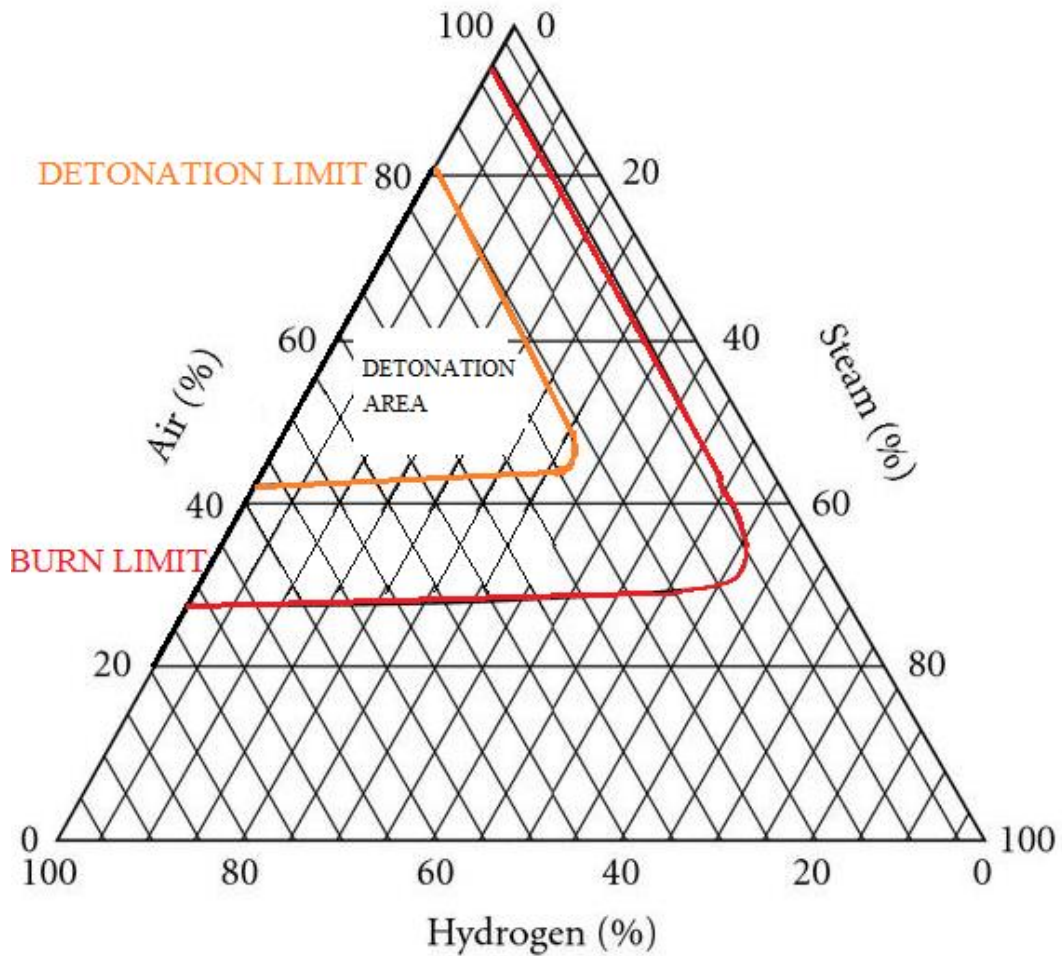


Figure 3. Shapiro flammability diagram (Kljenak, 2013)

2.2.2 Hydrogen Management in Severe Accident

Several measures have been studied and used in NPPS to prevent the build-up of explosive gaseous mixture of hydrogen in reactor containment. One widely used device for mitigating hydrogen explosion risk has been the passive autocatalytic recombiners (PAR). PAR's are used to remove hydrogen from the reactor containment by utilising the exothermal reaction between hydrogen and oxygen on catalytic surfaces generating steam and heat. The main reaction is described in Equation 4. (Payot et al. 2012, 2.) PARs are positioned to the containment in places in which the hydrogen accumulation is expected to occur. Figure 4 shows an example schematic of a PAR.



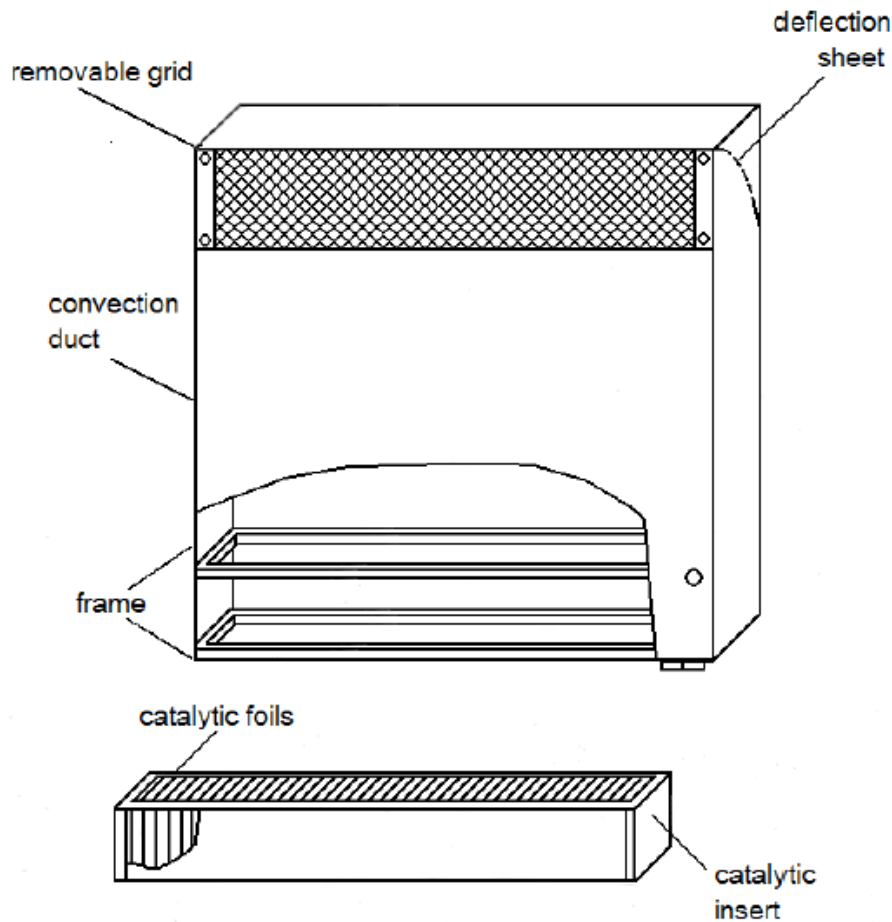


Figure 4. Example of passive autocatalytic recombiner (Kljenak 2013)

The advantages of PAR systems are the passive nature i.e. they operate without external power source, the ability to remove even small concentrations of hydrogen and no ignition is occurred i.e. the threat of fire is small. PARs can cope with a wide range of hydrogen release scenarios but they cannot handle rapid hydrogen generation of the worst cases. The effectiveness of PAR may be diminished with time due to the pollution of the catalytic surface. The containment geometry influences highly to the installation and the required location of the PARs. (OECD 1999, 25.)

Hydrogen combustion can be mitigated by igniting the hydrogen before its concentration becomes high enough to cause the risk of spontaneous detonation. The use of igniters can prevent the accumulation of hydrogen to the containment. The schematic of a hydrogen igniter is shown in Figure 5. (Kljenak 2013.)

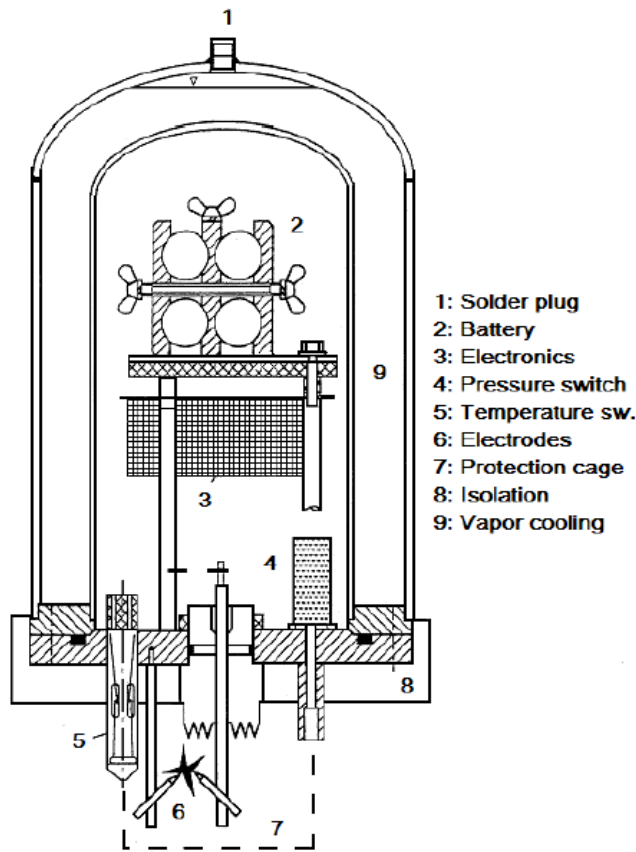


Figure 5. Schematic of a hydrogen igniter (Kljenak 2013)

The igniters can remove large quantities of hydrogen in very short times. The igniters should be used near the flammability limits to prevent damaging burns in the NPP. The disadvantages of the most igniters are the needs of electricity (excluding passive igniters) and the risk of burn propagation if the hydrogen concentration has risen to too high before ignition. (OECD 1999, 25.)

Hydrogen risk can be also mitigated by manipulating the containment atmosphere by different means. One of these means is to dilute the containment atmosphere with inert gas to mitigate energetic combustion regimes or even attain full inertization to suppress the combustion completely. Typical gases used in dilution process are carbon dioxide (CO_2) or nitrogen (N_2). (OECD 2000, 21.) The mitigation process, based on the post-inertization, has a major disadvantage: the timing is very critical and automated initialisation is not available, hence the operating personnel of the plant have to perform the initialisation of the inert gas injection (OECD 1999, 26). In the most commercial

BWR's such as Olkiluoto 1 and 2, the containment is permanently inerted by nitrogen to prevent the gas combustion and explosion hazard.

2.3 Hydrogen Distribution in Containment

High ranking phenomena affecting the gas distribution are gas transport, mixing, heat and mass transfer and inter-compartment flow processes (Auban et al. 2006, 1). It is essential to be able to predict the distribution of combustible gases inside the containment so that the function of mitigation and control systems can be assessed. For example, it is important that the systems are situated in the optimal spots in the containment. Mixing process has an important role on the way how combustible gases can accumulate and distribute inside the containment.

Mixing process can be defined as a process where fluids with distinguishable characteristics come together and form a fluid with a single characteristic. Mixing is an intra-compartment process and includes all phenomena in single open compartment or room. Temperature or constituent concentration can be the characteristic of the fluid. When mixing is incomplete a stratified condition is created (OECD 1999, 34.)

One hydrogen management technique is to guarantee effective mixing of containment atmosphere to prevent local hydrogen accumulation and formation of hydrogen rich regions. The mixing of the containment atmosphere can be achieved with many means. One of these is the actuation of containment sprays induce atmosphere mixing. Falling spray droplets from containment sprays induce convective gas flows in the containment atmosphere and mixing it. In an ice condenser containment, a feasible mixing method is to open all ice condenser doors to allow the main natural circulation flow within the containment. The natural circulation is achieved with hydrostatical pressure difference. The intention is that the flow pattern mixes the gas atmosphere so, that no high local hydrogen concentration can be formed. This is the hydrogen management method used in Loviisa NPP (Lundström 2001, 5).

One phenomenon that produces the mixing in the containment atmosphere is steam/gas injection sources to containment atmosphere. Injection flow with high momentum is

called jet and injection flow with lower momentum is called plume (Auban et al. 2006, 2). Jets and plumes coming e.g. from a break of the primary system can induce transport of steam and gas mixture between containment compartments affecting the wall condensation and hydrogen accumulation. These phenomena have been identified as playing important role in the safety of LWRs and also future IV reactors (Paladino et al. 2008, 1.) The effects caused by the jets and plumes depend on the transient scenario, location and injection direction (Auban et al. 2006, 2).

Over the last three decades, extensive studies on steam condensation on containment walls and structures have been performed. Studies have shown that the liquid films caused by the condensing steam have a strong influence on the condensation heat transfer (Andreani et al. 2010, 1, 20). The effect of the steam condensation to the distribution of gases and vice versa has to be considered. As the steam concentration decreases due to condensation processes, the concentration of non-condensable gases correspondingly increases and thus creating an additional thermal resistance that significantly decreases the condensation process. The steam condensation can also change the inert air-hydrogen-steam atmosphere into atmosphere where hydrogen burn or even detonation is possible.

The variables influencing the rate of condensation can be classified into three categories: primary variables, secondary variables and tertiary variables. The primary variables are the mass fraction of non-condensable gases, temperature difference and operation pressure. Secondary variables are the suction effect, mist formation and film waviness. Tertiary variables are the effect of the type of non-condensable gas (nitrogen, argon, helium and hydrogen) and the orientation of condensing surface. (Pappini et al. 2011, 4.)

3 CALCULATION METHODS

There are mainly two different types of methods used in the containment analyses: LP and field codes. LP method has been primarily used as the solution method in long-term SA analysis codes, because the simulation time is typically very long and fast simulation speed is required. (Povilaitis et al. 2011, 1.) Nowadays field codes are being used more frequently and put in practical use in containment analyses because the computer performance/cost ratio has increased lately. (OECD 1999, 113, 117.)

3.1 Lumped Parameter Method

Lumped parameter method is used in the most integrated/system codes that can be used to calculate all major aspects of in-vessel and ex-vessel phenomena including reactor coolant system and containment thermal hydraulic response, core heatup, core degradation and relocation and fission-product release and transport. Most of these codes use simplified physical models and conservation equations. (OECD 1999, 118.)

In a LP method spatially distributed field variables are replaced with single scalars within a chosen zone (Povilaitis et al. 2011, 2). This LP assumption states that in a control volume, differences of thermal hydraulic variables like temperature, density and concentration, are neglected and the time-dependent transport processes in the containment are presented with integral conservation equations. (OECD 1999, 118.)

In a system which is modelled via LP method, energy and mass are transported from node to node through branches. The momentum equations defined in branches determine the transported mass and energy. The LP method is one dimensional because the momentum equation is defined in the branch that has only one dimension, from a node A to a node B and nodes have no momentum associated with them. (OECD 1999, 119.)

Containment atmosphere is modelled with compartments usually called nodes or control volumes and flow paths (called branches in APROS) that connect the nodes together. Momentum equation is defined in branches and energy and mass conservation equations

are defined in the nodes. In order to solve the conservation equations numerically the equations must be discretised in respect to space and time, and the non-linear terms are linearized. In APROS, with the aid of mass and momentum equations a linear equation group, where node pressures are the only unknown variables, is obtained (Hänninen 2009, 25). By solving the matrix the unknown pressure can be defined.

3.1.1 General Advantages and Disadvantages of LP method

The important focus of LP codes in containment analysis has been the integrated analysis. In the integrated analysis, the behaviour of primary/secondary circuit and containment systems can be simulated simultaneously and the interactions and feedback of the systems can be taken into account. Usually LP codes have many interacting models for example thermal hydraulic, aerosol behaviour, fission product transport, engineering safety features, water distribution and other models related to design-basis accident (DBA) and SA. Due to ability to model and simulate many containment response related phenomena at the same time, LP codes are used e.g. to perform probabilistic risk and safety assessments (PRA, PSA) of SA scenarios. These studies require typically large number of sensitivity analysis and different scenario calculations. LP method is relatively fast-running on variety of platforms that is necessary feature in PRAs and PSAs, where a large amount of accident sequences have to be calculated. (OECD 1999, 120.)

The effort needed to create a plant input with a LP method is often lower than in field codes. LP codes are structured in a way that it is relatively easy to model different kinds of plant concepts/geometries and incorporate the related systems/models e.g. the engineering safety features to the input. LP method has been used for a long time and the validation base, user community and available experience are extensive. Resolution of the LP result is directly dependent on the accuracy of the input, because thermal hydraulic variables are presented in nodes by single scalar numbers. Also the molecular and turbulent diffusion modelling is generally lacking in LP methods. (OECD 1999, 120.)

3.2 Field Codes

Advanced containment codes with three-dimensional capabilities and computational fluid dynamics (CFD) codes are referred as field codes (Andreani et al. 2003, 2). In field codes the spatial variation of fluid properties is locally taken into account in the calculation. In the containment atmosphere, a momentum equation is solved at a number of discrete finite control volumes. Mass, energy and momentum conservation equations are developed on the basis of partial differential equations, where the trends in spatial variations of the calculated properties are accounted for inside a control volume. This calculation method requires a large number of control volumes to simulate the detailed behaviour of a thermal hydraulic system accurately. (OECD 1999, 119.)

Momentum equations in field codes are derived as multidimensional equations which consider the transfers from the connected control volumes and account for the advection of momentum between volumes. In field codes the viscosity divergence term in the Navier-Stokes equations can be calculated by the finite difference method. This, in theory, allows the prediction of non-homogeneous gas concentrations and temperatures within an atmosphere where the shear stress within a gas flow is important. (OECD 1999, 119.)

3.2.1 General Advantages and Disadvantages of Field Codes

Field codes are focused to predict the local and regional parameters of the system including concentrations, velocities and temperatures. If the modelling is done correctly the field codes can predict and determine primary and secondary flow patterns. Secondary flow is a relatively minor flow superimposed on primary flow. Flow patterns can be used to predict containment loads with a high degree of local accuracy. In field codes transport and combustion processes can be tightly coupled. Field codes are also useful in comparison calculations with LP thermal hydraulic models. (OECD 1999, 121.)

One of the main reasons, why field codes have not superseded the LP codes in containment analyses, is a relatively long computing time needed. Also the design time

of input set-up with the LP codes is much smaller. (Povilaitis et al. 2011, 2.) Performing sensitivity studies is very time consuming, because of the long computational times required. Other disadvantage of the field codes is the high sensitivity to user effect. The user choices on the complex input creation can have a great impact on the simulation results. Also numerical distortions can be amplified by the user. (OECD 1999, 121.)

4 CONTAINMENT CODES

Calculation codes have been used and developed since the mid-1980s for DBA and other safety and design analysis. The international co-operation of code development and verification in the containment code field has led to better understanding on the thermal hydraulic and gas-distribution phenomena taking place in containment. The prediction capabilities of the computer codes have become better and the more accurate results can be calculated with the aid of the better insight gained from the international co-operation. (OECD 1999, 113, 117.)

Thermal hydraulic containment codes are used in the decision making process. A variety of different safety calculations is needed in the design, licensing and safety improvement process of a NPP. Safety analyses done with computer codes include the whole accident scenario, from the initiating event to the possible environmental and other consequences. Codes are very useful tools when new accident mitigation devices are implemented. Results obtained from containment codes can be used to define the guidelines and system measurements for active and passive safety systems. (OECD 1999, 26.)

Containment codes are mainly used to calculate and predict the containment loading from DBA events, to make sure that the safety systems implemented in NPPs are adequate. The DBA-analyses are calculated conservatively, meaning that the thermal hydraulic variables that describe the containment behaviour such as pressure, temperature are calculated in a way that ensures that the sufficient safety margins are achieved. On the other hand, in the DBAs or SA analysis best estimate (BE) calculations methods are used in order to evaluate the risk. (OECD 1999, 27.) In BE calculations realistic input values and assumptions are used to enable as realistic description of the system phenomena as possible (IAEA 2009, 18).

To make sure that the analysis results of containment codes are correct, the codes must be validated and verified. Organization for Economic Co-operation and Development (OECD) has organised a number of International Standard Problems (ISP) to increase

the validity and accuracy of the codes used in nuclear safety research and assessments. (OECD 1999, 113.)

The overall performance of codes used in nuclear safety assessments and research can be evaluated by using three different indicators. These indicators are applicability, reliability and economics. The most important of these requirements is code applicability. The code must be able to reproduce the physical phenomena relevant to the behaviour of the system under review. The reliability of the codes can be determined by comparing the results given by the code to the results obtained by measurements. Because the thermal hydraulic behaviour of a system is a complicated matter, even though the codes analytical algorithms give accurate solutions, the predicted behaviour has uncertainties. The uncertainties are caused by simplifications, lack of physical modelling, empirical input variables and user input. (OECD 1999, 113.) Reliability of codes can be determined and developed with the aid of ISPs and code benchmark calculations, where the code results are compared qualitatively and quantitatively against measurements of separate and combined effect tests.

An additional requirement for containment codes is economics, especially when simulating long time SA phenomena in containment. The quicker the input can be build and the shorter computing time needed to simulate, the better. Containment codes designed to simulate SAs usually employ simple physic models without jeopardizing reactor safety. (OECD 1999, 113.)

4.1 Codes Applied in This Thesis

The APROS v.5.12.04 is used in the simulations in this thesis. Comparison of the APROS six-equation and the APROS LP containment package codes is performed by modelling identical scenarios. The main objective is to compare the two different calculation models and determine the impact of the convection term used in six-equation model. Two simple test cases are performed to gain knowledge of the performance of the models. To discover the differences, a more complicated hydrogen transport and mixing experiment HM-2 conducted at THAI-test facility, is modelled

with both codes. The investigated APROS codes are described in Chapter 4.1.1 and 4.1.2.

APROS is a multi-purpose process simulator program developed originally by VTT and Imatran Voima Oy. The development of APROS started in 1986. Nowadays the program is developed and owned by VTT Technical Research Centre of Finland and Fortum Nuclear Services Ltd. The APROS program simulates e.g. thermal hydraulic processes in NPPs and conventional power plants. (Hänninen & Ylijoki 2008, 15.)

The APROS program has three different thermal hydraulic models that can simulate two-phase flow. The models are a homogeneous model, five-equation drift-flux model and six-equation two fluid model. The most sophisticated thermal hydraulic model of APROS is the six-equation model. (Hänninen & Ylijoki 2008, 15.) APROS has also a LP containment package developed especially to calculate the thermal hydraulic phenomena inside containment system during postulated accidents.

4.1.1 APROS Six-equation Model

The APROS six-equation model is a separate one-dimensional two-phase flow solver that can simulate systems with separate gas and liquid phases. The system is governed by six partial differential equations. (Hänninen & Ylijoki 2008, 15.) These equations are conservation equations of mass, momentum and total energy of liquid and steam phases. These equations are presented as follows:

$$\frac{\partial \alpha_k \rho_k}{\partial t} + \frac{\partial \alpha_k \rho_k u_k}{\partial z} = \Gamma_k \quad (5)$$

$$\frac{\partial \alpha_k \rho_k u_k}{\partial t} + \frac{\partial \alpha_k \rho_k u_k^2}{\partial z} + \alpha_k \frac{\partial p}{\partial z} = \Gamma_k u_{ik} + \alpha_k \rho_k \vec{g} + F_{wk} + F_{ik} + f_k(v, pu, fl) \quad (6)$$

$$\frac{\partial \alpha_k \rho_k h_k}{\partial t} + \frac{\partial \alpha_k \rho_k u_k h_k}{\partial z} = \alpha_k \frac{\partial p}{\partial t} + \Gamma_k h_{ik} + q_{ik} + q_{wk} + F_{ik} u_{ik} + \alpha_k \rho_k u_k \vec{g} \quad (7)$$

Equation 5 is the mass conservation equation, 6 is the momentum conservation equation and 7 is the energy conservation equation. Here k stands for the phase (liquid or gas), α

for the volume fraction, ρ for the density, u for the velocity, t for the time, z for the space coordinate, Γ for the mass change rate, i for the interface of phases, w for the wall of a flow channel, \vec{g} for the acceleration of gravity in the flow direction, F for the friction force, the function f_k in the momentum equation takes into account the effects of valves, pumps and form loss coefficients describing different obstacles in the flow channel, h is the specific enthalpy, p is the pressure and q is the heat flow. (Hänninen & Ylijoki, 2008, 17.)

If the gas phase includes non-condensable gases, such as hydrogen, nitrogen or oxygen, the conservation equation for the non-condensable gases is needed. The six-equation model of APROS can also treat non-condensable gases that are dissolved in the liquid phase. The conservation equation of non-condensable gases is presented in equation 8.

$$\frac{\partial(\alpha_g \rho_{nc})}{\partial t} + \frac{\partial(\alpha_k \rho_{nc} u_g)}{\partial z} = 0 \quad (8)$$

Here g stands for the gas phase and nc stands for the non-condensable gas.

The flow geometries in APROS are defined as nodes and branches. Node is a control volume with a defined length and cross-sectional area. Two successive nodes are connected to each other with a flow path called branch. The pressures, void fractions and enthalpies are solved in nodes and the velocities are calculated in the branches. (Hänninen et Ylijoki, 2008, 15) This means that APROS uses staggered grid: different variables are calculated over different grids. The staggered grid discretisation scheme is illustrated in Figure 6.

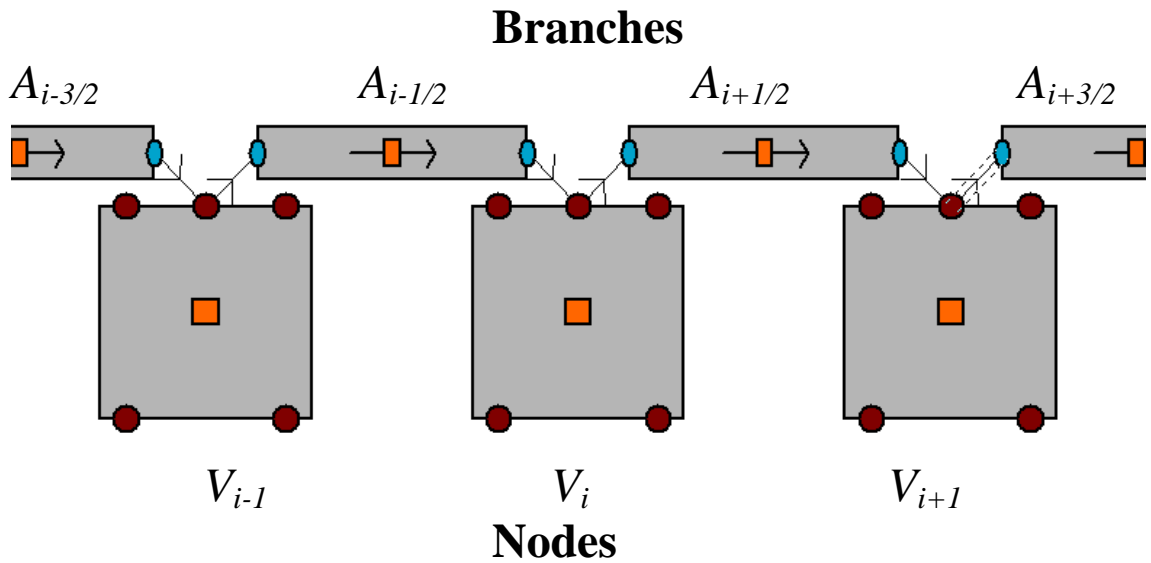


Figure 6. The staggered grid discretisation scheme used by APROS

Numerical solution of flow systems is gained by discretising the equations 5, 6, 7 and 8 in respect to time and space and the terms must be linearized. The values for the terms F_w (wall friction), F_i (interfacial friction), q_i (interfacial heat transfer) and q_w (wall heat transfer) are calculated from the empirical engineering correlations. These terms have a great effect on the thermal hydraulic solution. (Hänninen & Ylijoki 2008, 17.) The equations are solved iteratively until the mass error of both the gas and liquid phases becomes acceptably small.

4.1.2 APROS Containment Model

The NPP containment model of APROS is developed to model thermal hydraulic conditions and phenomena in the containment during different states of reactor accident scenarios. Also some chemical processes, such as hydrogen combustion can be treated with the model. Also modelling of the engineering safety features, and accident management hardware is included.

The containment model applies the LP method approach. In the LP method the gas region of a certain node is assumed to be homogeneous gas mixture of non-condensable gases and water vapour. The containment node may include the gas phase, fog i.e. water droplet phase and a sump i.e. water pool. The APROS term “sump” is used to describe all kinds of water pools in the containment. Water droplets of the fog phase can be

formed in node due to condensation of supersaturated steam or as a result of direct water injection to the node gas region.

The thermal hydraulic system of the containment model is described with the differential equations of the mass, momentum and energy. The mass balance equation 9 is needed for the pressure solution, momentum equation 10 is needed for the calculation of the mass flow rate between the nodes and the average temperature in nodes is calculated with the energy balance derived from equation 11. (Silde & Ylijoki 2013, 10)

$$\frac{\partial A\rho}{\partial t} + \frac{\partial A\rho w}{\partial z} = S_i \quad (9)$$

$$\frac{\partial A\rho w}{\partial t} + \frac{A\partial p}{\partial z} = S_j \quad (10)$$

$$\frac{\partial A\rho h}{\partial t} + \frac{\partial A\rho wh}{\partial z} = S_k \quad (11)$$

Here the symbol w is the velocity of mixture and the right side terms S_i , S_j and S_k of the equations describe the sources of mass, momentum and energy.

The containment can be divided into arbitrary number of nodes which are connected with gas and water branches. Most important engineered safety features like internal and external spray systems, ice condenser and suppression pool system including vent pipes can be modelled if necessary. Sources to the containment can be specified either by using the own source modules, where the injection properties can be specified by input tables, or alternatively by using a direct connection to the thermal hydraulic calculation in the primary or secondary systems.

5 THAI FACILITY

The THAI test facility, located in Germany, is a technical-scale plant of nuclear reactor containment. The THAI facility has been operated since 1998 by Becker Technologies in close co-operation with AREVA NP and Gesellschaft für Anlagen- und Reaktorsicherheit (GRS). The main objective of the THAI facility is to provide an experimental database for validation of LP and CFD containment codes. Typical experiments performed in THAI facility include stratification, distribution and depletion effects. (Allelein et al. 2008, 5.)

At the THAI facility, typical safety relevant thermal hydraulic phenomena occurring in containment during SA can be investigated in the separate and combined effect tests. These include turbulent free convection and stagnant stratified containment atmospheres which can be combined with hydrogen, iodine and aerosol issues. (THAI Program 2013, 3.)

The volume of the THAI test vessel is 60m^3 and it is made of 22 mm thick stainless steel. The test vessel is thermally insulated. The height of the test vessel is 9.2 m and diameter is 3.2 m. The diameter of the lower end of the facility, called sump room, is 1.4 m. The outer vertical walls of the facility are subdivided in to three vertical sections that can be heated or cooled to adjust and control the thermodynamic properties of the containment atmosphere. The THAI test vessel can be operated up to 180 °C temperature and 14 bar pressure. (THAI Program 2013, 3; Burkhardt et al., 2009, 1.) The THAI test vessel is presented in Figure 7.

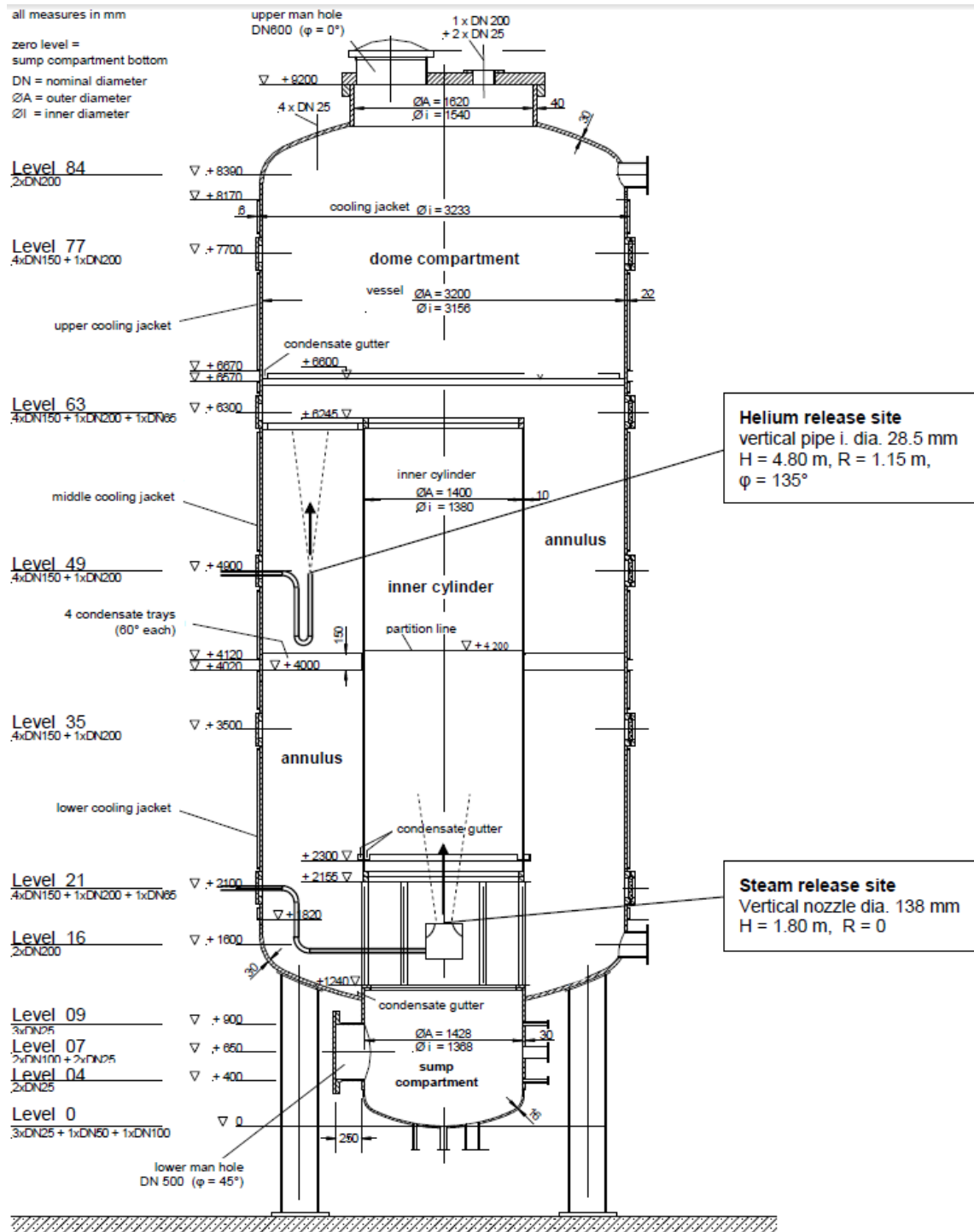


Figure 7. THAI test vessel (THAI Program, 2008, 15)

The THAI test vessel is insulated by rock wool with a thickness of 120 mm (OECD-NEA 2010, 1). Inside the THAI test vessel the inner cylinder is mounted between the heights of 2.3 – 6.2 m. The inner cylinder is made of 10 mm thick stainless steel with an outer diameter of 1.4 m. Also condensation trays can be mounted in the annular area of the test vessel. (Funke et al. 2012, 2) The condensation rates of the test vessels inner

walls can be defined by measuring the condensed liquid collected in the condensation trays.

5.1 Instrumentation of the THAI Facility

The THAI facility is equipped by the innovative measuring, sampling and data acquisition systems. The thermal hydraulic conditions are monitored with a comprehensive conventional instrumentation for temperature, pressure, dew points and wall condensation rates.

THAI provides experimental database for validating LP and CFD codes. Especially the CFD codes require very comprehensive measurements in order to verify the reliability of the code. To gain comprehensive measurement data, the instrumentation of THAI covers state of the art and advanced sensors and methods, especially for field measurements, in-line gas- and aerosol diagnostics, on-line and offline. The typical instrumentation of THAI vessel is presented in Figure 8. (THAI Program 2013, 4.)

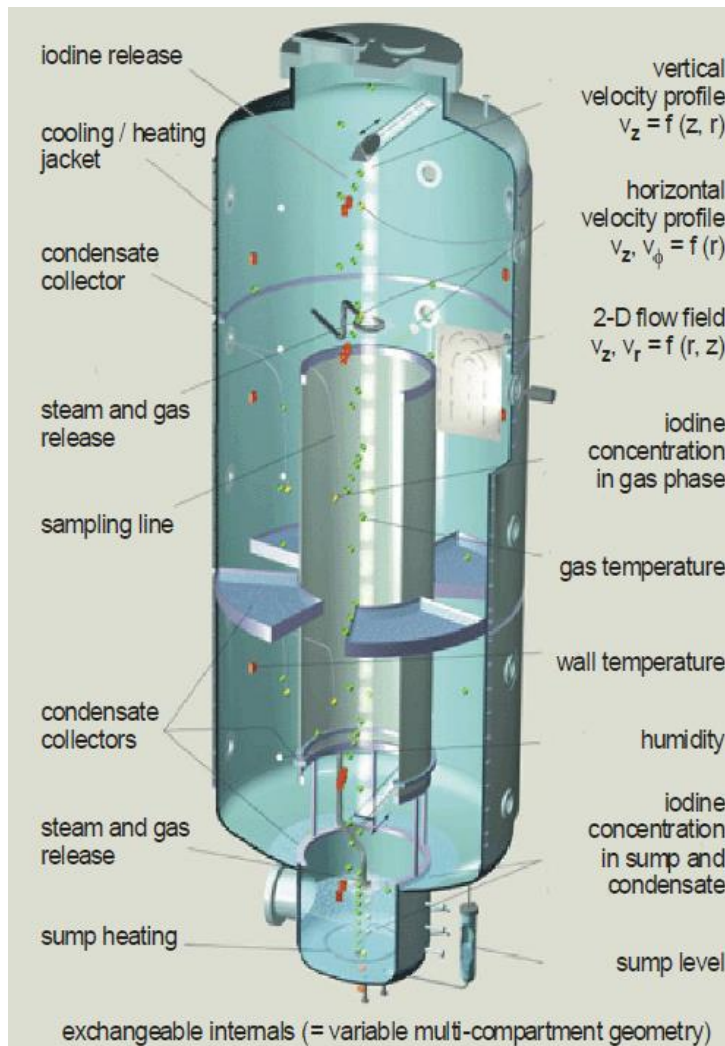


Figure 8. Typical instrumentation of THAI vessel (THAI Program 2013, 4)

Steam can be injected to the test vessel up to maximum rate of $35 \frac{\text{g}}{\text{s}}$. The steam is generated by the separate steam generator and injected into the vessel. (Funke et al., 2012, 2.) The main distinguishable feature of the THAI facility is the coupling of thermal hydraulics, fission product transport and chemistry, especially for iodine with its high radiological importance. Generation and feeding techniques for soluble and insoluble aerosols and radioactive marked iodine are applied. Iodine measurements and chemical analysis are supported by the Radiochemical Laboratory of AREVA NP as engineering service. (THAI Program 2013, 2-4.)

6 SIMULATIONS OF SIMPLE TEST CASES AND HM-2 EXPERIMENT

The containment analyses with the containment codes can be divided into two parts. In the first part the input of the simulation has to be prepared. The main task during the setup process of the simulation is the nodalisation of the calculation problem. The nodalisation describes the physical attributes of the calculation problem to the calculation model. Initial values, geometric values and boundary conditions need to be calculated and described to the code input before the simulation. After the systems code input has been developed, the simulation can be started. The second part of the analyses is the analysis of the simulation results.

The simulations in this study are divided into two parts. In the first part two simple test cases are simulated to gain knowledge from the effect of the numerical diffusion and effect of mass error in gas stratification calculations and the effect of the convection term in six-equation model of APROS to the node differential pressures in a large break test case. In the second part of the simulations the THAI HM-2 hydrogen stratification and mixing experiment is calculated with APROS six-equation model and containment model and the results are compared and analysed.

6.1 Simple Test Cases

In the first test case a simple hydrogen stratification problem is calculated with the APROS six-equation model. The aim of this this test case is to provide useful information from the effect that mass error and numerical diffusion has on the results of hydrogen stratification. In the second test case, containment pressure loads are calculated with the APROS containment model and the APROS six-equation model. The calculations of the six-equation model are performed with and without the modelling of the momentum transfer i.e. the convection term in the momentum conservation equation. The source data to the containment used represent approximately a typical steam release in a guillotine steam line break of pressurised water reactor (PWR).

6.1.1 Effect of Mass Error and Numerical Diffusion

The purpose of the first test case is to study the suitability of APROS six-equation model to calculate non-condensable gas stratification in containment atmosphere. In addition, possible effect of numerical diffusion on stratification is studied. Because no containment calculations involving more than one non-condensable gas have been calculated earlier using APROS six-equation model, it was decided to simulate a simple stratification case using a simple nodalisation. The purpose of the test is to verify that the APROS six-equation model is suitable for calculation of stratification phenomena in the more complicated geometry of the THAI facility.

The model of the first test case consists of 20 nodes and 28 branches and it describes an enclosed volume of 1.28 m^3 with a height of 4 m. This nodalisation represents the modelling concept, where the open space of containment compartment is divided into several sub-nodes, to enable flows between cells. The containment is initially filled with nitrogen at ambient pressure (0.1 MPa) and temperature (20.7 °C). Hot hydrogen (126 °C) is injected into the top nodes for 2 seconds with a total mass flow of $0.2 \frac{\text{kg}}{\text{s}}$. After the hydrogen injection phase the hydrogen stratification is formed and the injection is stopped. Then the system is simulated for 9998 seconds to see how the stratification is sustained. The nodalisation of the first test case is presented in Figure 9. The system is assumed to be adiabatic i.e. no heat structure are modelled.

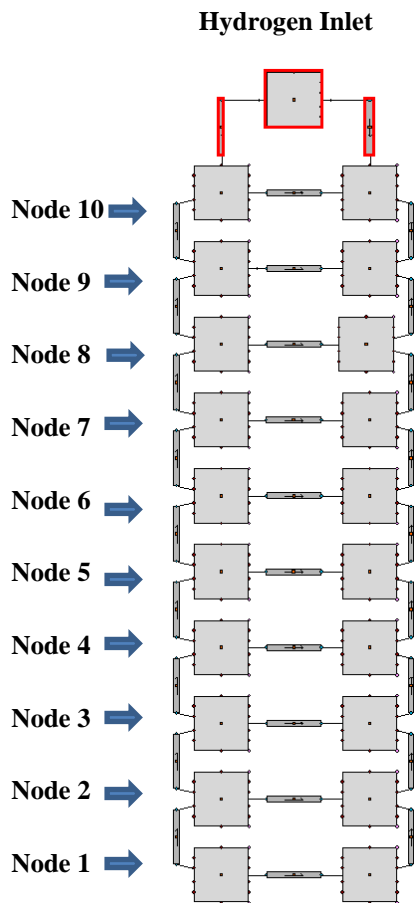


Figure 9. Nodalisation used in the mass error test case

The thermohydraulic models of APROS are developed originally to simulate the two phase flow of water in situations, where amount of non-condensable gases is relatively small. Hence it could be challenging to simulate containment phenomena, where the amount of non-condensable gases is very high.

The mass error in the containment stratification calculation is studied with two different calculations. The input used in the calculations are otherwise identical, except that the variable defining the minimum iteration cycles used in every time step was varied between three and seven. Figure 10 and Figure 11 present the results of the simulations.

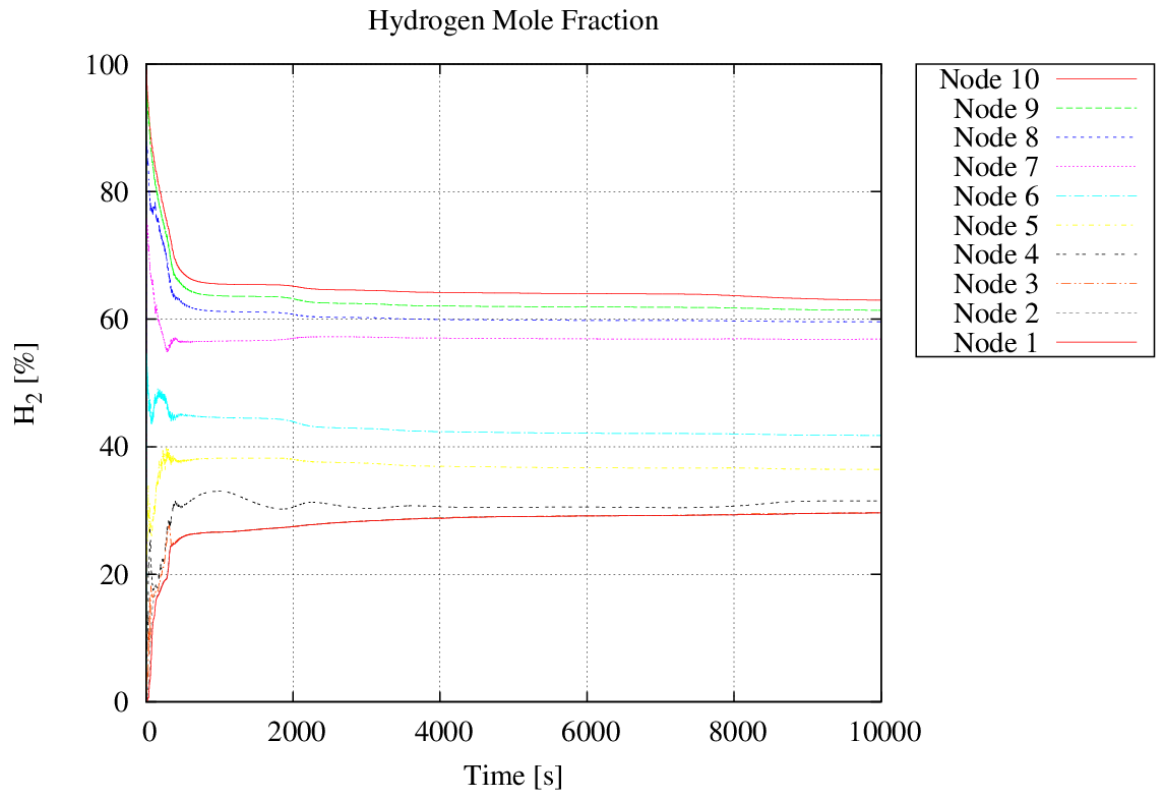


Figure 10. Results of the first test case using minimum iteration number of three

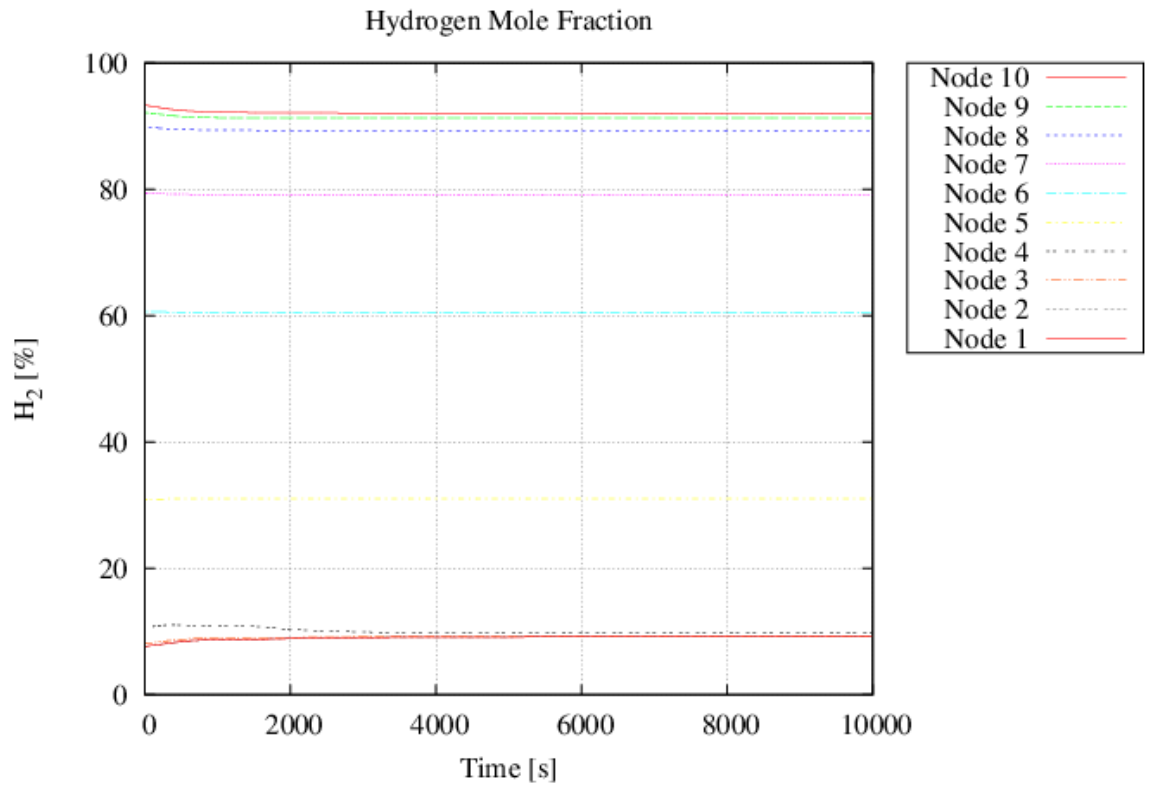


Figure 11. Results of the first test case using minimum iteration number of seven

The simulation results with the minimum iterations cycles of three shows, that after the hydrogen injection is stopped the hydrogen is mixed with the nitrogen in the atmosphere of the containment due to gas flows induced by mass error. Because the density of hydrogen is much smaller than the density of nitrogen, it is reasonable to assume that the hydrogen would form a relatively stable layer on the top of the containment.

As seen from the results, an increase in the minimum iteration cycle number has a large impact on the results of the simulation, because the mixing induced by the mass error decreases. The same results can be obtained by decreasing the allowed mass error criteria of non-condensable gases which can be defined in the APROS code. It is evident that as number of iteration increases, the mass error causing nonphysical mixing to the simulation decreases.

The six-equation model uses first order upwind scheme with averaged concentrations and temperatures in the nodes. This feature creates numerical diffusion which makes sharp concentration and temperature distributions nonphysically smoothed when the fluid proceeds over several calculation nodes. The effect of numerical diffusion is studied by using the same nodalisation as previously in the exception that in the beginning the nodes are filled with cold water (20 °C), and the hydrogen injection is replaced by hot water (90 °C) injection $20 \frac{\text{kg}}{\text{s}}$. This is due the fact that six-equation model of APROS is able to use second order upwind scheme in the liquid enthalpy calculation. Figure 12 and Figure 13 presents the temperature profiles of the numerical diffusion test case.

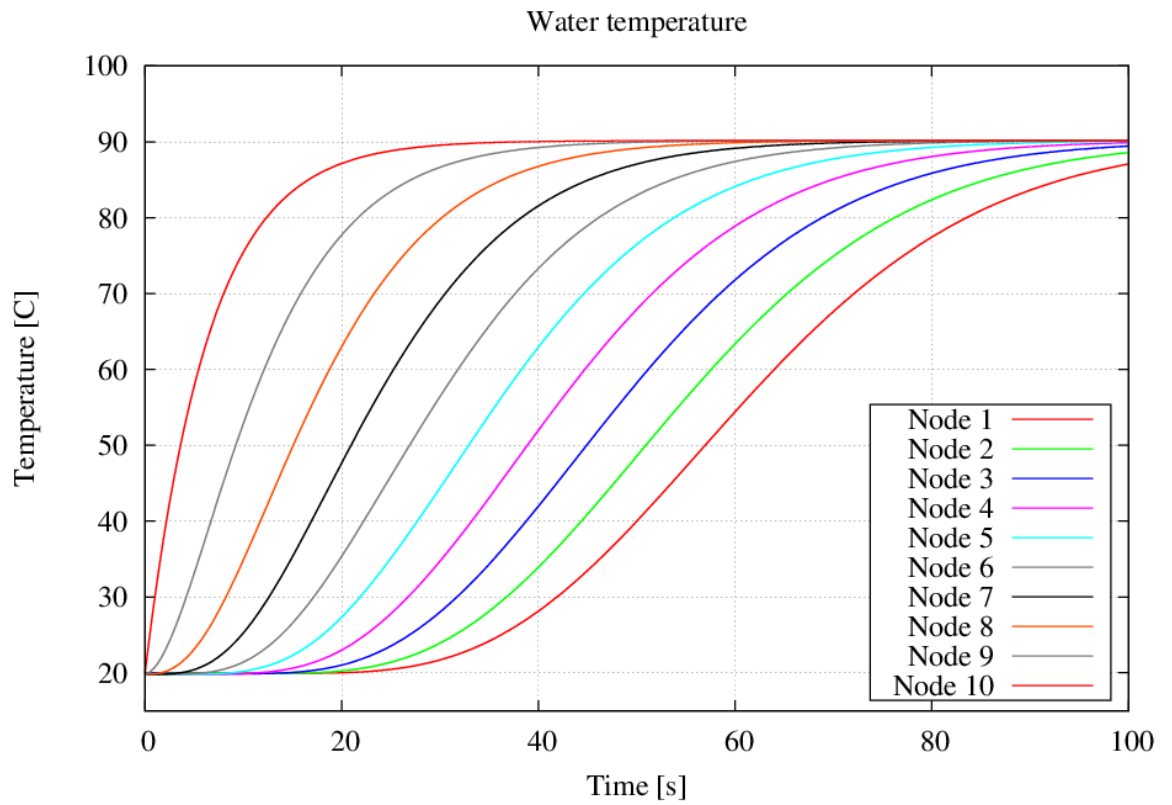


Figure 12. Results of numerical diffusion study using first order upwind scheme

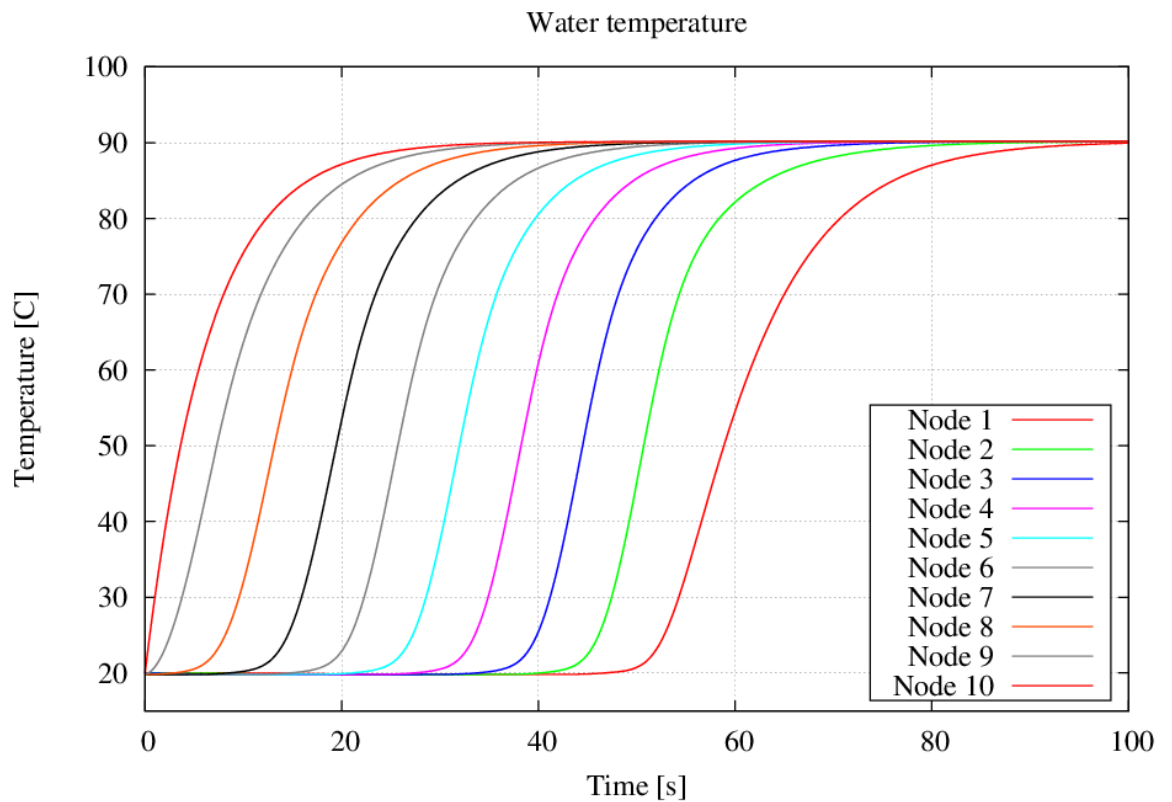


Figure 13. Results of numerical diffusion study using second order upwind scheme

The simulation results show a noticeable improvement in the sharpness of the temperature gradient. When the first order upwind scheme is used the temperature of the bottom node starts to rise at 25 s and the temperature of the middle node is close to 40. In the second order upwind scheme simulation the temperature of the bottom node starts to rise at 50 s and the temperature of the middle node is 90 °C.

As seen from the calculation results the use of second order upwind scheme improves clearly the simulation results of the sharp temperature front. It can be concluded from the results of these simulations that it would be beneficial if possible to add the second order upwind scheme to the gas concentration calculation procedures of both the APROS six-equation model and the containment package.

6.1.2 Momentum Transfer

The purpose of this test case is to study the effect the momentum transfer option has in the simulation of containment pressure loading. Especially the pressure differences of nodes are examined. The nodalisation used in this test case describes approximately one steam generator compartment and the upper volume of a PWR containment. The total volume of the model is 47100 m³, in which 2100 m³ describes the steam generator compartment. The steam mass flow to the containment is approximately the same as a mass flow of a main steam line break. In this test case generic (PWR) containment is pressurised as a consequence of a guillotine steam line break. The steam line break is assumed to take place in the bottom of a steam generator compartment. This assumption is not in line with the typical design of a PWR, but because of the academic nature of this test case the assumption is reasonable. The test case is calculated with the APROS containment model and the six-equation model. The effect of the momentum transfer option of the six-equation model is also studied.

During a break of pressurised pipe inside a compartment, the pressure differential across the compartment wall will reach a maximum value within a short time, which is typically less than five seconds. The peak differential pressure is primary determined by the inertia of the injected fluid in and around the openings of the containment, wall friction in the flow channel and by the flow resistance through the openings. The

containment of NPP is designed to sustain and reduce the pressure increase caused by an accident. Heat transfer and condensation on the walls and structures of the containment has a substantial role in the pressure decrease during accident, but the impact on the peak differential pressure is minor due to very short time to the peak. (Mitsubishi 2008, 28.)

The constructed models of the APROS containment package and the six-equation model are as identical as possible. The model consists of nine nodes and eight branches. No heat structures are modelled. The nodalisation is presented in Figure 14. The nodes one through seven represents the steam generator compartment of the PWR containment. Node eight represents the dome of the upper compartment and node nine other parts of the upper compartment.

In the beginning of the case the containment is filled with air and the atmosphere is at ambient pressure and temperature (0.1 MPa, 24 °C). During the postulated accident scenario steam (mass flow: $5000 \frac{\text{kg}}{\text{s}}$, enthalpy: $2800 \frac{\text{kJ}}{\text{kg}}$) is injected to the bottom of the steam generator compartment.

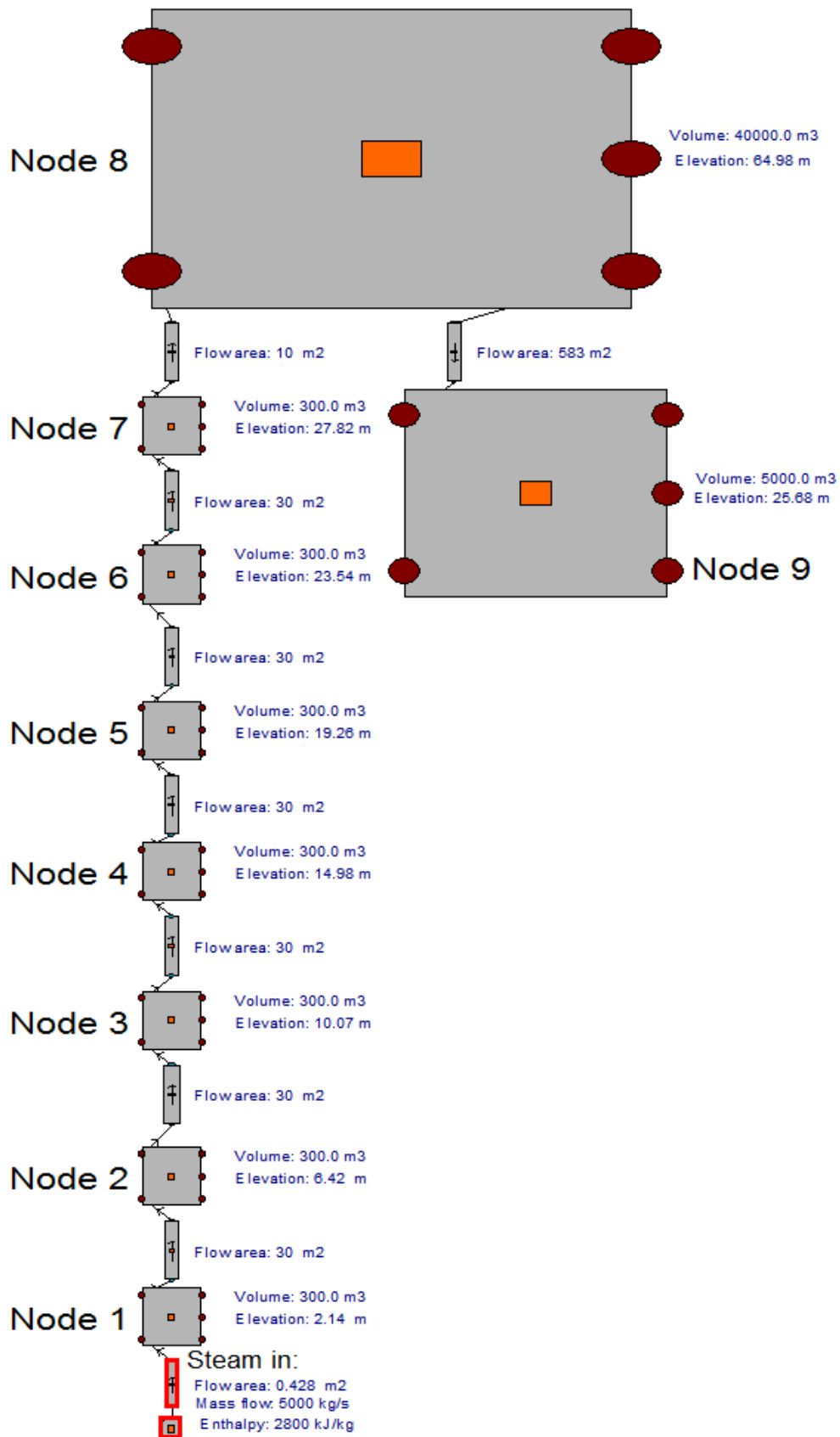


Figure 14. Nodalisation of the generic containment used in the momentum transfer test

In the six-equation model of APROS, it is possible to choose an option to include the convection term in the momentum conservation equation. The convection term is the second term ($\frac{\partial \alpha_k \rho_k u_k^2}{\partial z}$) in the momentum balance equation of APROS thermal hydraulic model (see Eq. 6).

When the momentum transfer option is activated in the branches connected to a node, the incoming momentum flow is distributed between all branches where the flow is leaving the node. The incoming momentum flux is distributed to the leaving branches according to the areas of the branches. (Hänninen & Ylijoki 2008, 31.)

In the six-equation model the option of calculation mode of velocity was changed from the default value of 0 to 1 in the nodes 8 and 9. If the attribute has the value 0, the node velocities are calculated from branch velocities, taking into account those branches which transfer the momentum flux. If the attribute has the value 1, the phase velocities are calculated on the basis of the node phase mass flows. Mass flows are converted to velocities using the flow area of the node. It was necessary to change the option to perform the simulations, to prevent excessive condensation. Node velocities are taken into account when calculating bulk condensation when steam is flowing into a cold volume.

The simulation model was designed in a way that the effect of momentum transfer term was assumed to be possible strong, but still realistic. The Figure 15, Figure 16 and Figure 17 present the simulated pressures of the nodes calculated with the APROS six-equation model and the containment model.

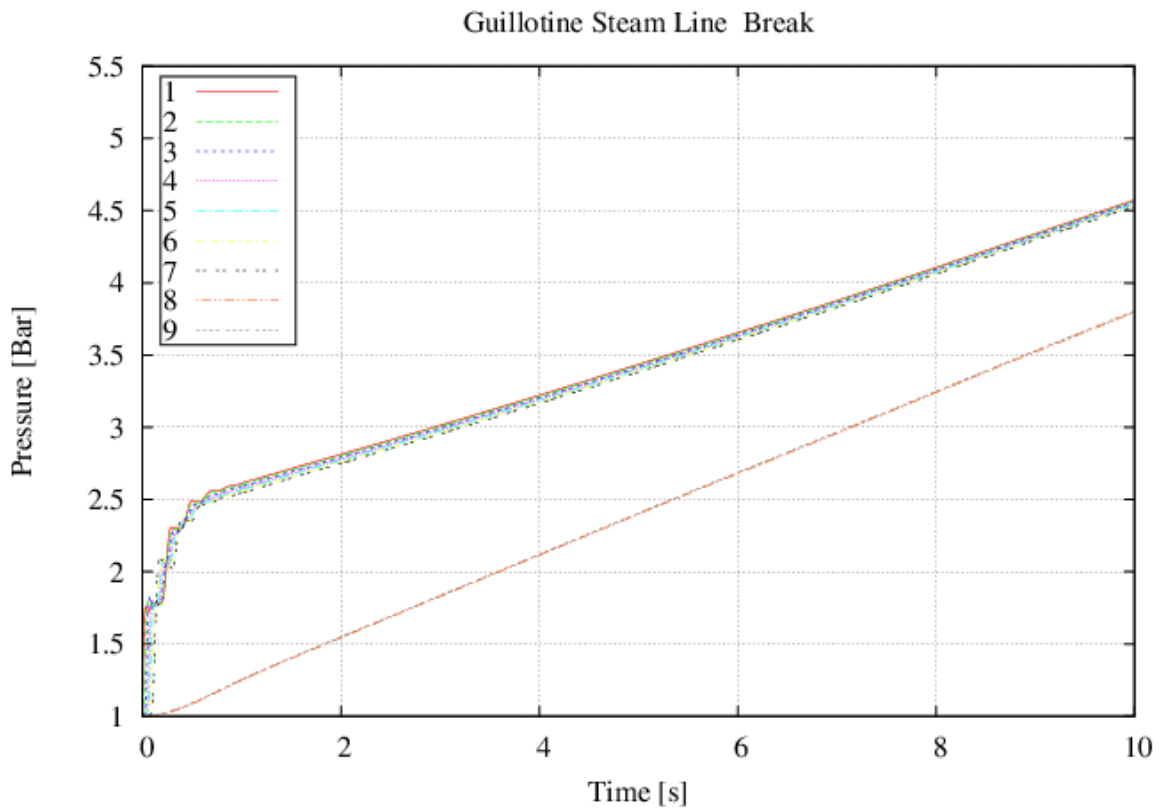


Figure 15. Pressures of the containment calculated with 6-equation model no momentum transfer

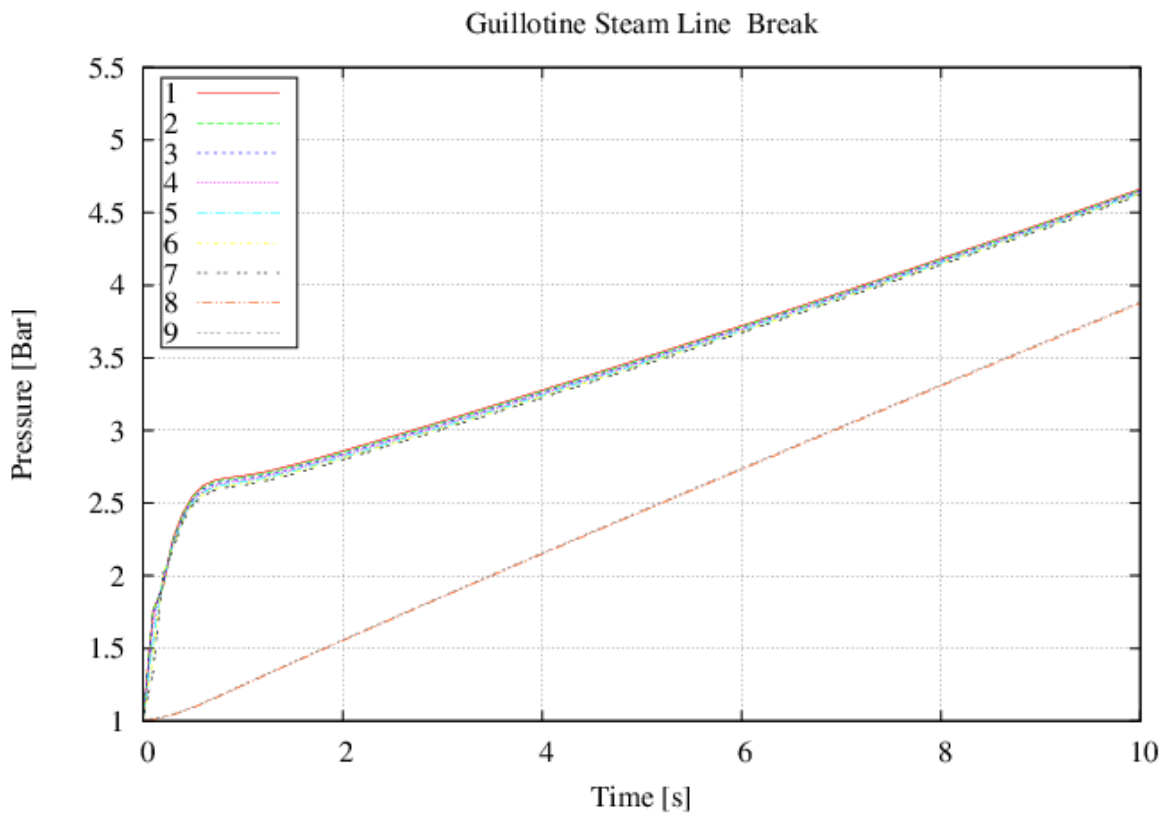


Figure 16. Pressures of the containment calculated with the containment model

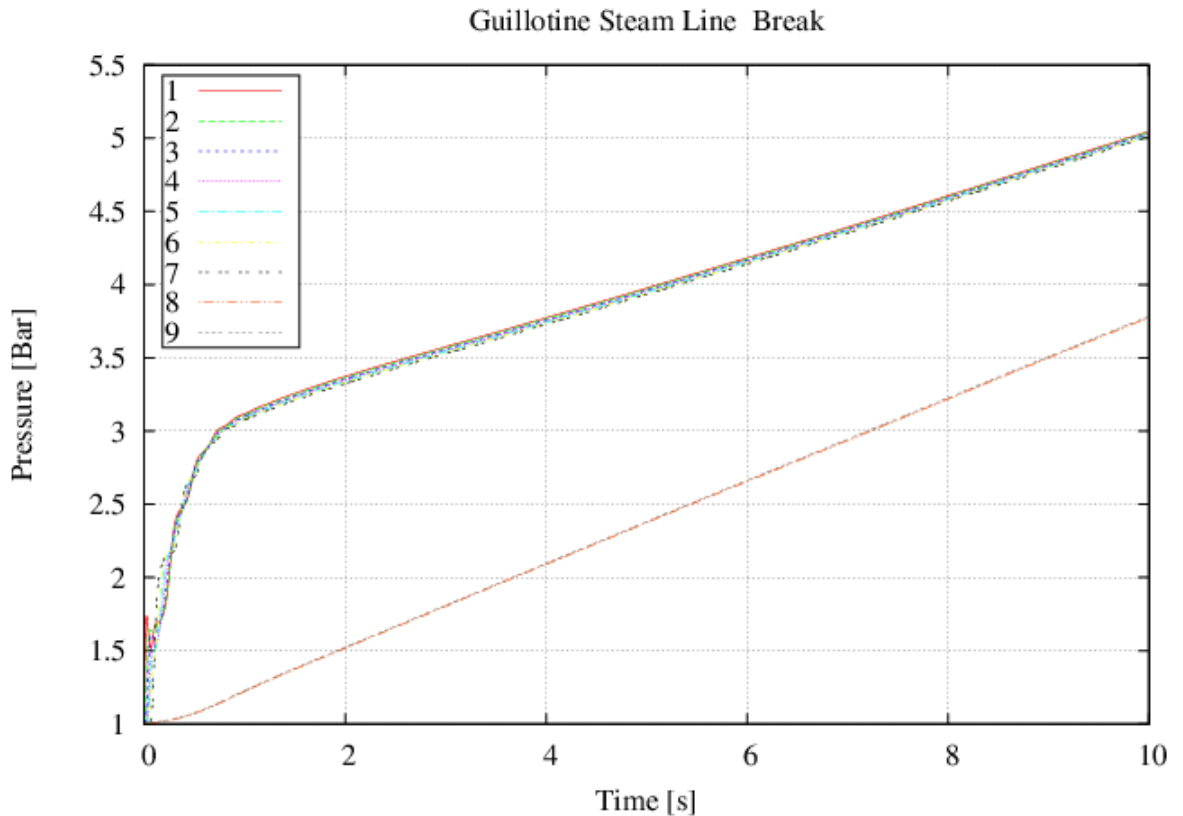


Figure 17. Pressures of the containment calculated with 6-equation model using momentum transfer

As the steam injection begins, the pressure of the steam generator compartment starts to rise rapidly. The pressure increase of the steam generator compartment stabilises after the steam flow reaches the large volume of the containment dome. The calculated pressure histories are almost identical using the containment model and the six-equation model as expected. When the momentum transfer is used in the six-equation model, the pressure in the steam generator compartment raises almost 50 kPa higher than in the other simulations. The pressure stays higher during the whole simulation.

The differences between the simulations can be easily observed when studying the pressure differences of the nodes. The most interesting results are the pressure difference between the nodes 7 and 8. The flow area is reduced from the 30 m² of the steam generator compartment to 10 m² that describes the flow area of the alleged rupture disc between the steam generator compartment and the upper volume of the containment. The form loss coefficients of the branches connecting the steam generator nodes were set to the value of 0.1 in order to model small flow obstacles inside the steam generator room. The form loss coefficient of the branch simulating the rupture

disc between the steam generator compartment and the upper compartment was set to the value of 1.5 to describe the choking of the flow area. The simulated pressure differences are presented in **Error! Reference source not found.**

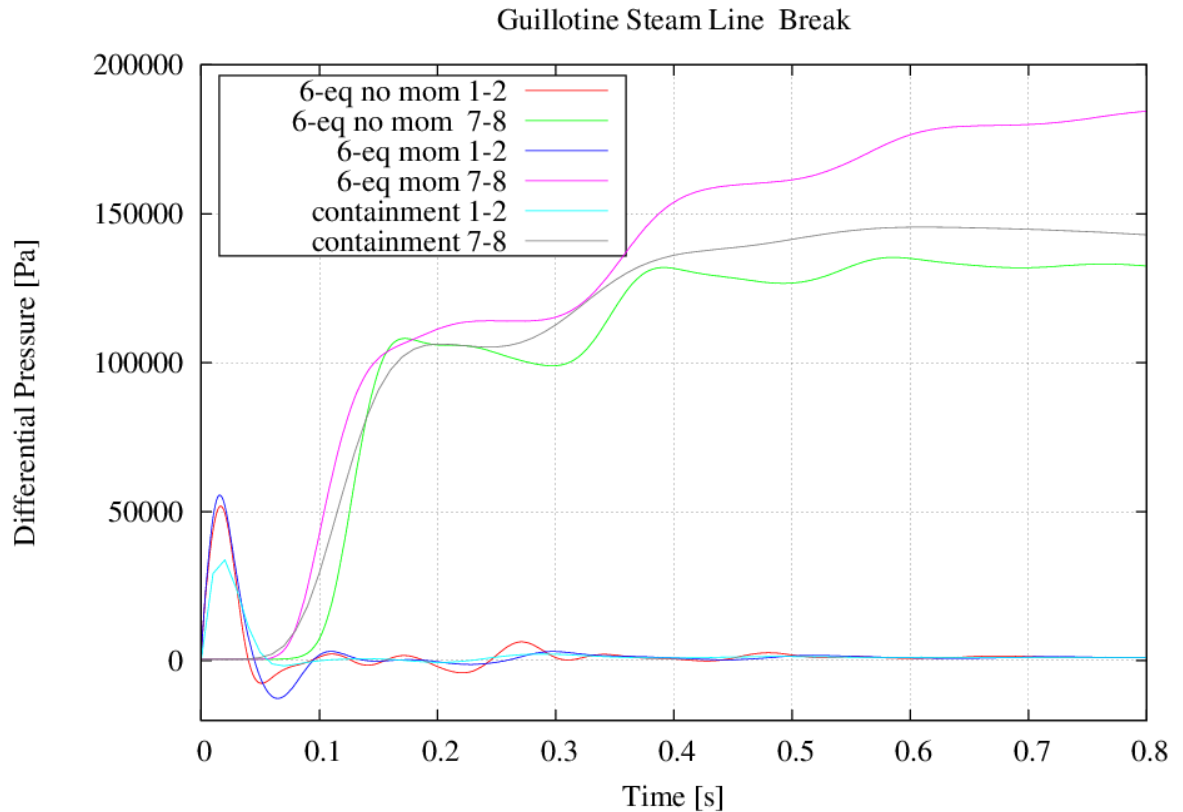


Figure 18. Pressure differences of nodes 1-2 and 7-8

The pressure difference history between nodes seven and eight behaves quite similar in the simulations of both codes, but in the six-equation model using the momentum transfer, the pressure difference is 50 kPa higher starting from the 0.3 s, than in the other simulations. Because no measurement data is available from the experiment the only conclusion from this test case is that the momentum transfer has some effect on the simulation results, but it is uncertain if the results predict the physical behaviour better or worse. This matter should be studied in more detail.

6.2 THAI HM-2 Experiment

The HM-2 experiment was a part of the OECD-THAI project. The objective of the OECD-THAI project was to gain knowledge of the behaviour of hydrogen, iodine and

aerosols in the containment of LWRs during SA. The project also provided experimental data for ISP to improve and validate the advanced LP- and CFD- codes used in reactor applications. (THAI Program 2010, 18.)

The HM-2 experiment is the second experiment of the two experiment HM-test setup. In the HM-test setup erosion of a stable atmospheric stratification layer by a buoyant plume from below was investigated. In the most of the available hydrogen distribution experiments, helium has been used as a substitute for hydrogen in order to guarantee safety of the experiment process. One of the main objectives of the HM-test setup was to verify the assumption of the transferability of the helium and hydrogen in distribution problems. The other objective was to generate extended data base for the code validation calculations. Experiments HM-1 and HM-2 are almost identical gas stratification and mixing experiments performed at the THAI facility. The experimental procedure used in both experiments is a simplified version of the ISP-47-Part 2 test, which is considered to be very sensitive to gas distribution phenomena (Fischer et al. 2005). In the experiment HM-1 helium is fed to the THAI vessel to gain stratified gas atmosphere, whereas in HM-2 hydrogen is used instead of helium. (THAI Program 2010, 18.)

HM-2 experiment used a detailed instrumentation to gain information from the light-gas distribution, especially the phenomena leading to the gradual dissolution of the hydrogen stratification layer in the upper part of the test vessel. (THAI Program 2008, 8.)

6.2.1 Test Configuration and Procedure of the HM-2 experiment

The HM-2 experiment can be divided into two separate phases. In the beginning of the experiment the THAI vessel was filled with nitrogen and the atmosphere was at ambient pressure and temperature (1 bar, 21 °c). The first phase, where hydrogen was injected into the test vessel from a nozzle at level of 4.8 m, took 4200 seconds. The injected hydrogen formed a hydrogen-rich cloud above the release nozzle. The hydrogen volume concentration was approximately 37 % in the upper part of the vessel in the end of the first phase. The second phase started two minutes after the first phase. In the second

phase steam was injected from the lower plenum of the test vessel below the inner cylinder. The steam injection was started at 4320 s and stopped at 6820 s. (THAI Program 2008, 22.)

During the first injection phase, steam was added to the hydrogen injection as a tracer. The steam formed fog droplets within the cold hydrogen flow. The fog droplets acted as tracer particles and the flow profile of the hydrogen injection was formed. The droplet flow was measured with a Laser Doppler Anemometry (LDA). (THAI Program 2008, 28.) The configuration of the THAI-test vessel is presented in Figure 19.

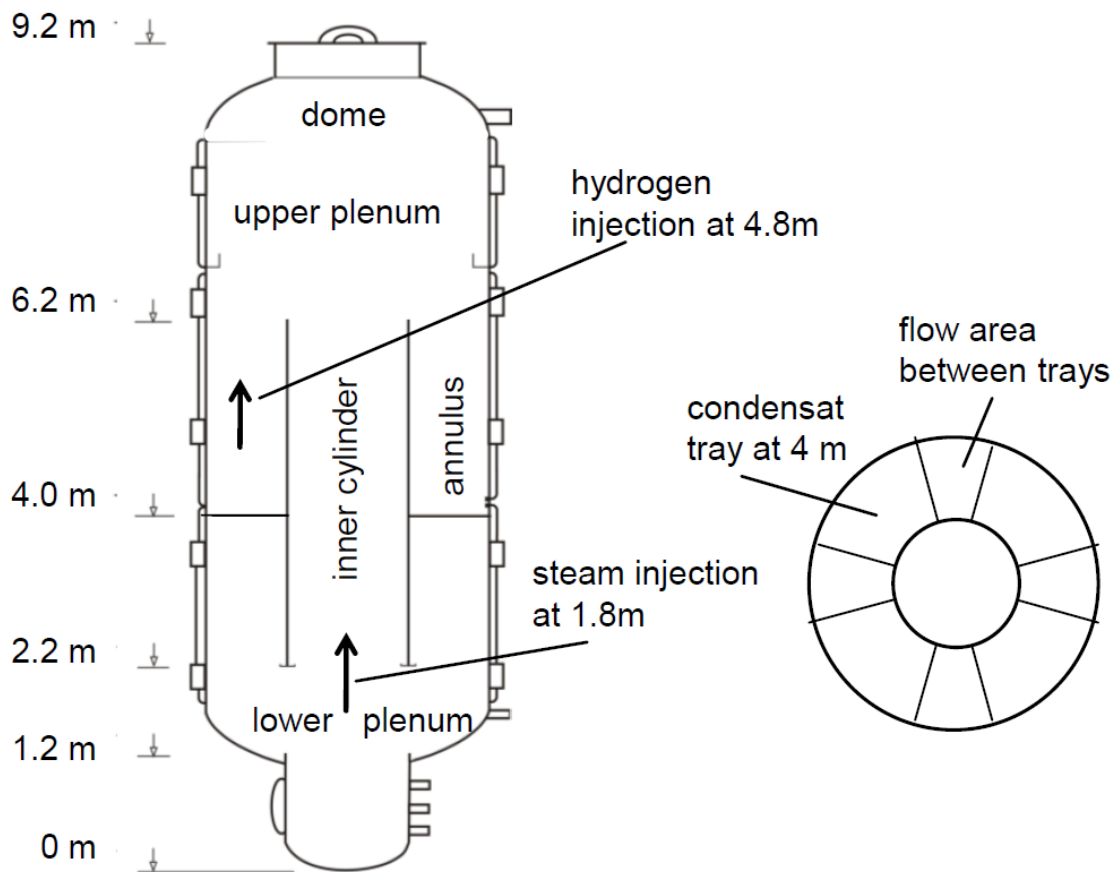


Figure 19. THAI vessel configuration of HM tests (OECD-NEA, 2010, 2)

The hydrogen and steam injected to the test vessel from a vertically installed nozzle with a diameter of 28.5 mm and 138 mm, respectively. The temperature of the injected hydrogen was approximately 60 °C and the steam was injected into the facility at 110 °C. The injection mass flows are presented in Figure 20. (THAI Program 2008, 9)

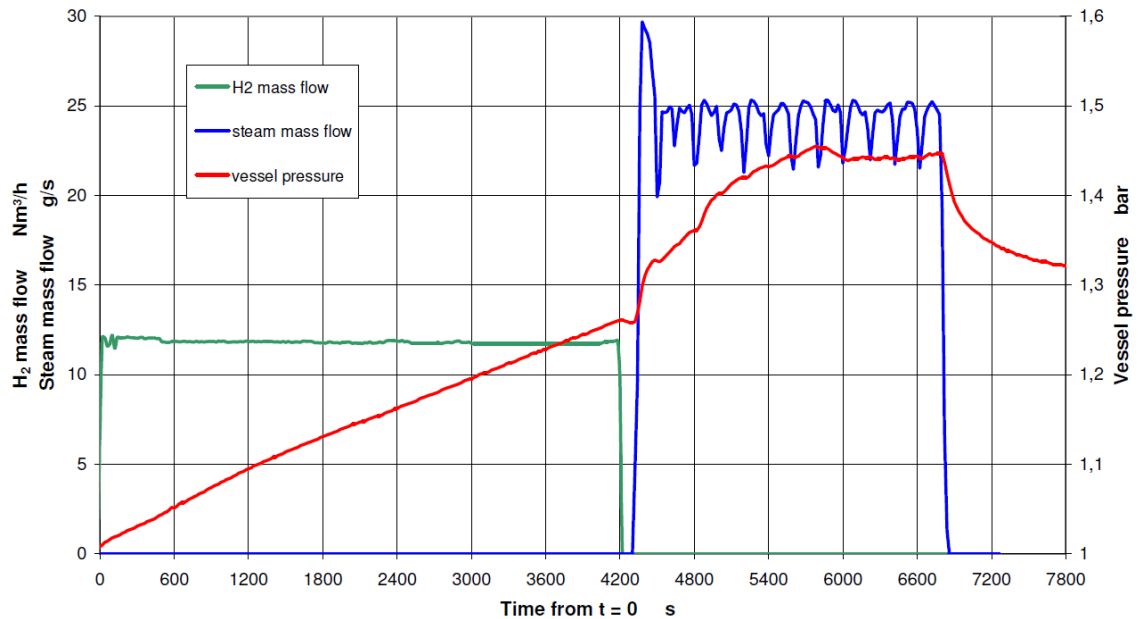


Figure 20. Hydrogen and steam mass flow and resulting pressure of the HM-2 experiment (THAI Program 2008, 29)

6.3 Nodalisation of the THAI Facility

In LP approach, it is important to design the nodalisation with utmost care and utilise the means to circumvent the known limitations of the method. User has a strong impact on the calculation results. The ‘user-effect’ was confirmed in the OECD/CSNI ISP-47 benchmark on containment thermal hydraulics, where the best and the worst results was achieved by the same LP code but different users (Kelm et al. 2013, 2).

Containment analyses done with LP containment codes have been traditionally made using a coarse nodalisation, where one node represents a whole room or a compartment of the containment. It is not possible to simulate gas distribution process using this standard nodalisation scheme. During the last years, capability of the LP codes to model the gas distribution processes has been studied by using a novel method of dividing the containment compartments into a several sub-nodes. (Burkhardt et al. 2009; Kljenak & Mavko 2010; Malet et al. 2010; Povilaitis et al. 2011)

In order to simulate gas stratification and dissolution of a gas cloud with LP codes, the vertical distribution of the containment nodes should be detailed enough. The radial

node resolution does not have a notable influence on the calculation results, if the gas distribution problem is a volume symmetric with respect to the vertical axis. Otherwise it is useful to divide the modelled volume respect to the vertical area. If the problem involves rising gas/steam plume or jet, it is recommended to add to the model a special nodalisation in the injection zone. (Schwarz et al. 2011, 6; Povilaitis et al. 2011, 10)

The THAI facility was modelled with the APROS six-equation model and the containment model. The constructed models are as identical as possible to enable a thorough comparison of the models. The nodalisation of the THAI facility is composed of 144 nodes, 111 heat structures and 340 branches. The nodalisation was divided to 28 vertical levels in order to simulate the gas distribution properly. The annulus area of the THAI facility is divided into four parts. Nodalisation of the THAI facility is shown in Figure 21.

The nodalisation consists of five stacks of nodes in vertical direction. The hydrogen injection nozzle is modelled in the stack number one. Stack number two describes the volumes in the centre axis of the THAI facility, with the same diameter as the inner cylinder. The annular volume of the test vessel is divided into four parts. Stacks four and five are adjacent to the stack one. Stack three is an opposite side from stack one on the other side of the central stack.

The bold red lines in the Figure 21 represents the walls of the inner cylinder. Therefore, between the vertical levels four to ten only the flow paths indicated by red arrows in the radial cross section of the nodalisation are modelled. The outer walls of the test vessel and the walls of the inner cylinder are modelled by 111 heat structures. The outer walls are insulated with a rock wool.

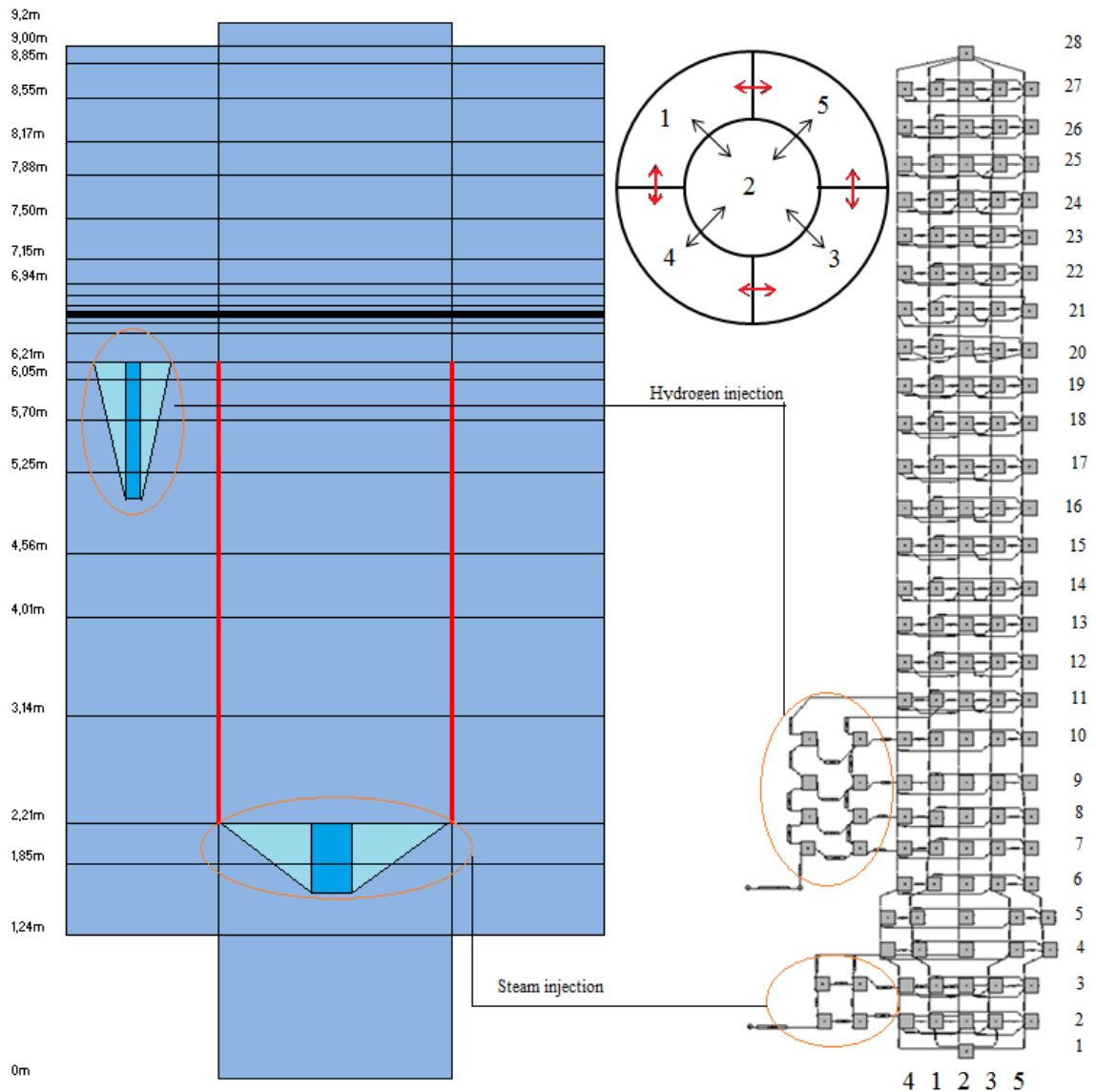


Figure 21. Sketch of the test facility (left) and APROS nodalisation (right)

6.3.1 Nodalisation of the Injection Zones

The knowledge gained from previous gas stratification and mixing experiments calculated with APROS and other LP codes has given a strong indication that a special nodalisation scheme is needed to be able to model physical flow behaviour of a rising plume or a jet. (Burkhardt et al. 2009, 7)

As seen from the Figure 21, special attention is given in the modelling of hydrogen and steam injection zones. The hydrogen and steam injection zones are modelled using eight

and four nodes, respectively. A schematic Figure of the used nodalisation utilised in the injection zone modelling is presented in the Figure 22.

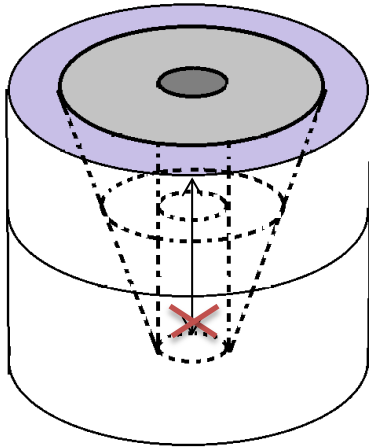


Figure 22. Schematic of the nodalisation used for the modelling of the injection zones

The core of the injection zone is modelled by a cylinder shaped node with a diameter same as the injection nozzle surrounded by a cone shaped node. The cylinder and cone shaped nodes are inside the main node of the modelled volume.

6.4 Simulation Considerations of the HM-2 Experiment

The THAI experiment HM-2 was chosen to be calculated in this master's thesis to verify the capability of the APROS six-equation model and the containment model in modelling hydrogen stratification and dilution of gas mixture if steam, nitrogen and hydrogen. Even though the HM-2 experiment does not represent any specific transient scenario and containment setup, it can give valuable information on the reliability of the calculation procedures utilised by the codes.

The APROS six-equation model is mainly designed to model two phase 1-D pipe flow in NPP applications. Therefore, in order to simulate the containment experiments with large amount of non-condensable gases some additional considerations need to be taken into account. The APROS six-equation model is designed for simulating various kinds of processes and it has many input options/settings that could affect the simulation results. In the following Chapters the effects of some of the major setting is described and also the effect of the injection zone nodalisation is shown.

6.4.1 Condensation Correlation

The APROS six-equation model has several alternative condensation correlations. These are Shah correlation, Chen correlation, Nusselt theory for condensation on the outer surface of tube banks and Nusselt theory for condensation inside a horizontal pipe. In this thesis, the HM-2 experiment was simulated using both the Shah correlation and Chen correlation with the Vierow-Schrock correction that reduces the interfacial heat transfer when non-condensable gas is present. The simulation results with different correlations are compared to the measured pressure history in the Figure 23.

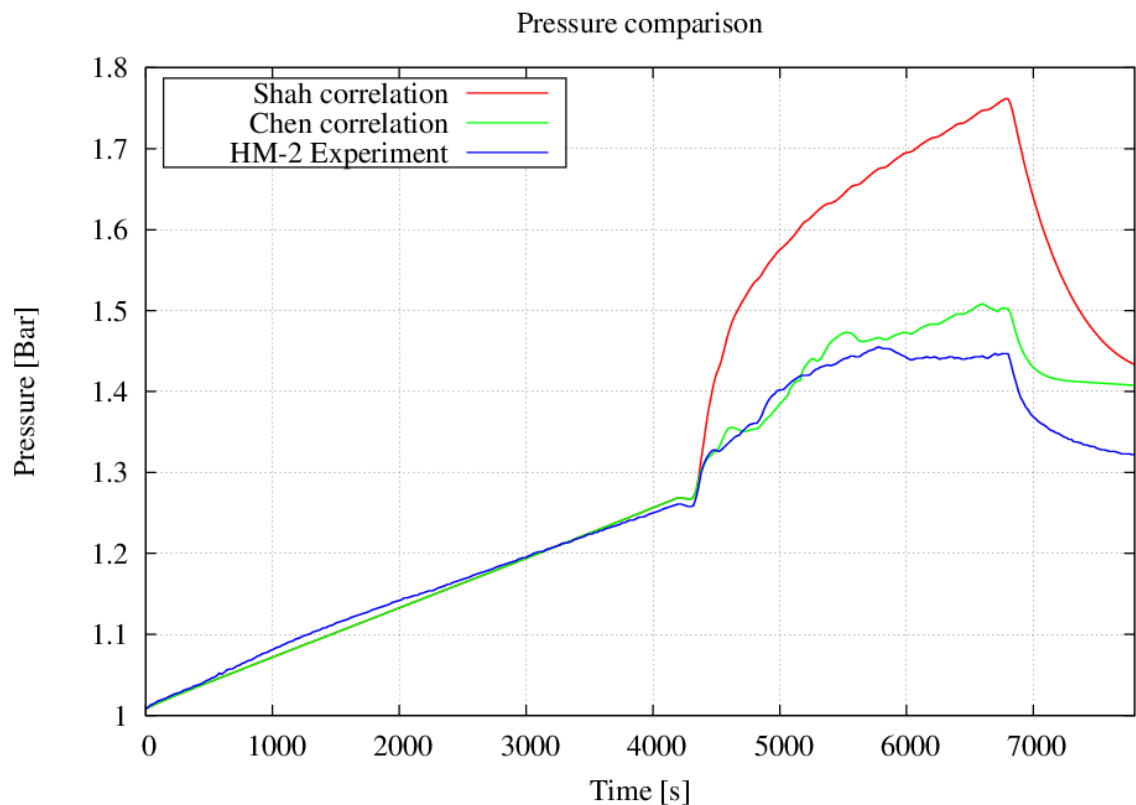


Figure 23. HM-2 experiments calculated and measured pressure history

It can be concluded from the results that the Chen condensation correlation is more suitable for this kind of problem. This empirical conclusion is confirmed by the fact that the Chen correlation is valid for co-current annular-film flow inside vertical and horizontal tubes (Hänninen & Ylijoki, 2009, 34). With these reasons, there is a clear reason to use the Chen correlation in the simulations of this thesis.

6.4.2 Number of Minimum Iterations

In the Chapter 6.1.1 it was concluded that the minimum iteration calculation cycles have a major impact on the mass error and gas stratification calculations when using the APROS six-equation thermal hydraulic model. Because the nodalisation used in the test case was simplified, e.g. no heat structures were modelled, it was decided to calculate the HM-2 experiment using value of 3, 5, 7 and 9 for the minimum number of iterations to find out the impact on calculation results. The histories of simulated hydrogen mole fraction in the nodes located in the top and bottom of the test vessel are presented in the Figure 24. The first number of the legend is the number of minimum iterations, second number describes the vertical level and the third number the horizontal location of the node, respectively.

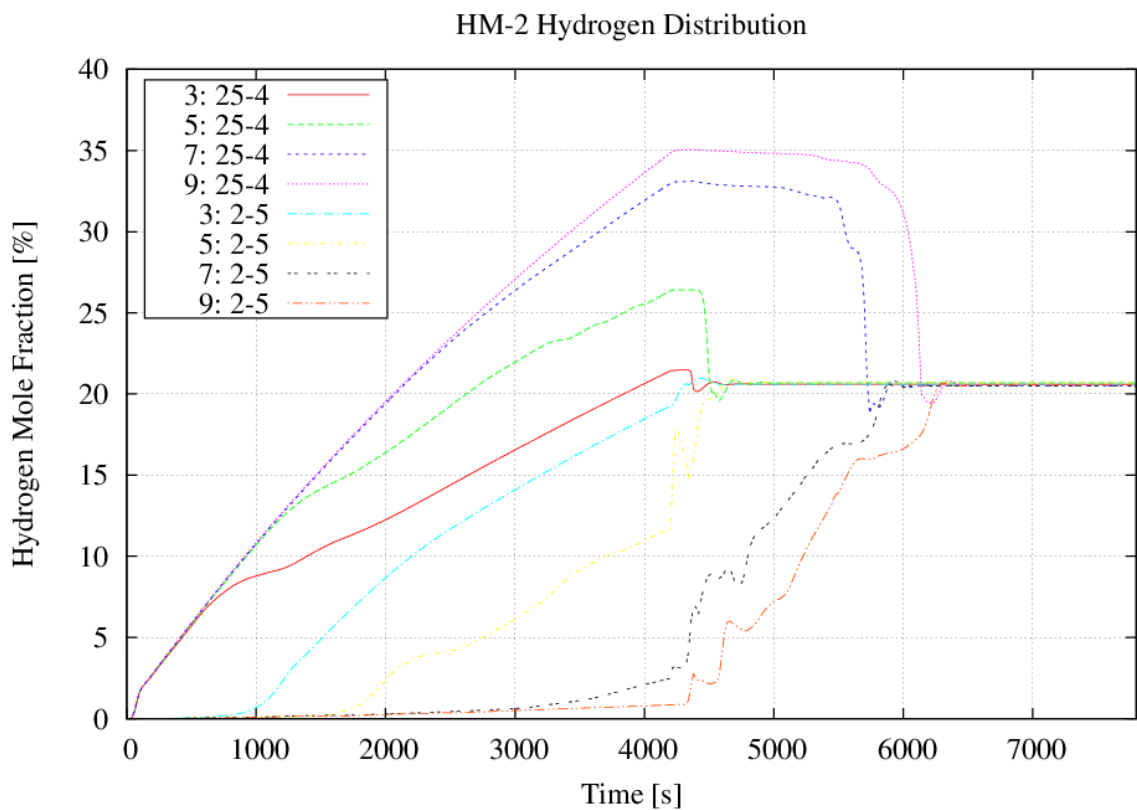


Figure 24. Distribution of hydrogen calculated with APROS 6-equation model using minimum iterations of 3, 5, 7 and 9

As seen from the calculation results the minimum iteration cycles has a significant influence on the calculation results. When minimum number of iteration cycles is small (3), hydrogen is mixed completely in the atmosphere even before the steam injection

has started at 4200 s. In case of five minimum iterations, the hydrogen is relatively stratified before the steam injection, but as soon as the steam injection starts the atmosphere is mixed very rapidly.

The overall behaviour of the hydrogen mixing and stratification is quite consistent in the case of seven and nine minimum iterations, but some deviations still exist. It was concluded that using at least nine or more iteration cycles, the mass error becomes small enough to get reasonable and accurate results. The upcoming simulations use nine simulation iteration cycles.

6.4.3 Momentum Transfer

One of the interesting features of the APROS thermal hydraulic model is the ability to transfer and distribute the incoming momentum flux to the leaving branches. This feature is not included in the LP containment model of APROS. Thus, the influence of the momentum transfer on the calculation of hydrogen stratification was studied.

The HM-2 experiment was simulated with the APROS six-equation model using three different assumptions: 1) momentum transfer is not activated at all, 2) momentum transfer is activated in all vertical branches during the whole simulation, and 3) momentum transfer is activated only in the vertical branches of the special injection nodes during the hydrogen and steam injection phases. The calculation results are seen in the Figure 25, Figure 26 and Figure 27.

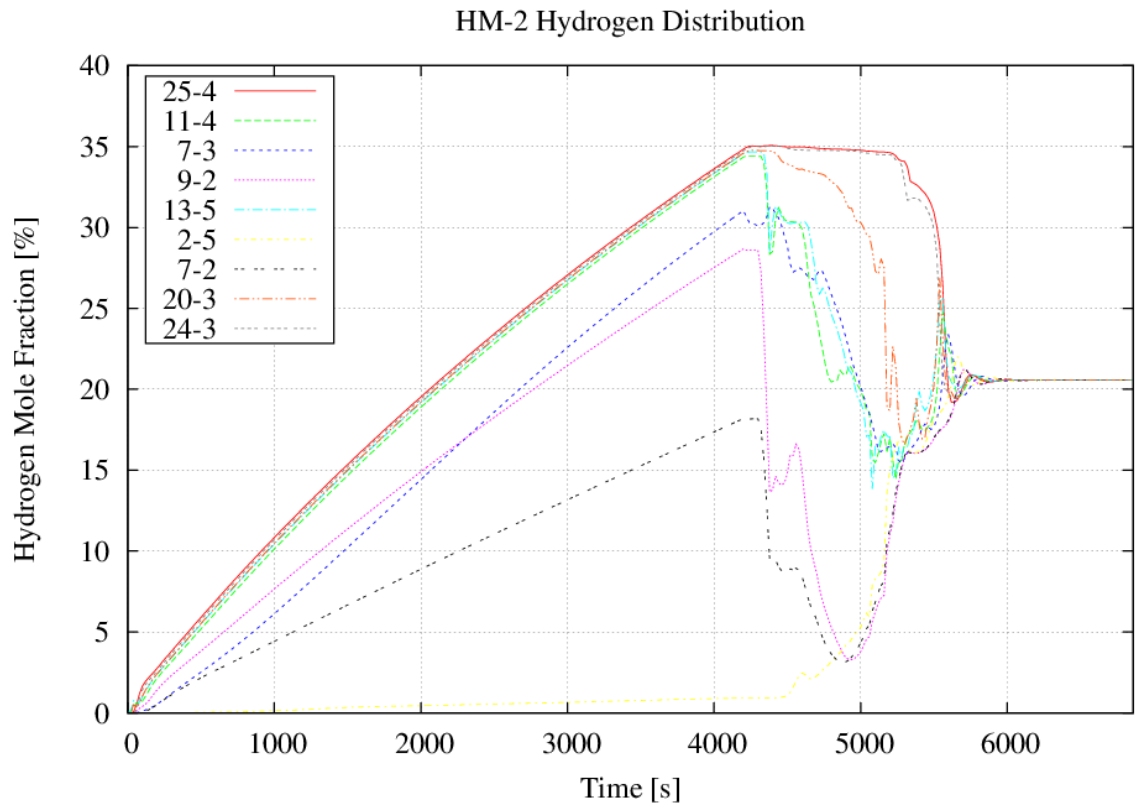


Figure 25. Hydrogen distribution calculated with APROS 6-equation model without momentum transfer

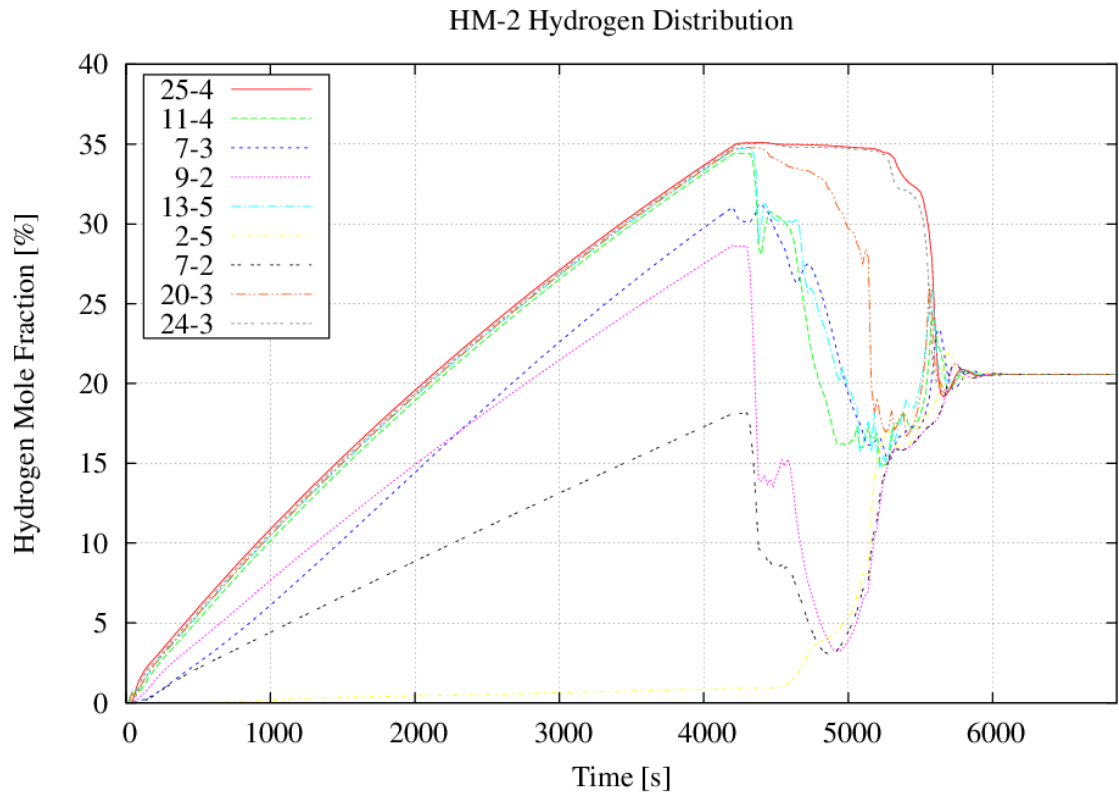


Figure 26. Hydrogen distribution calculated with APROS 6-equation model using momentum transfer in the vertical branches

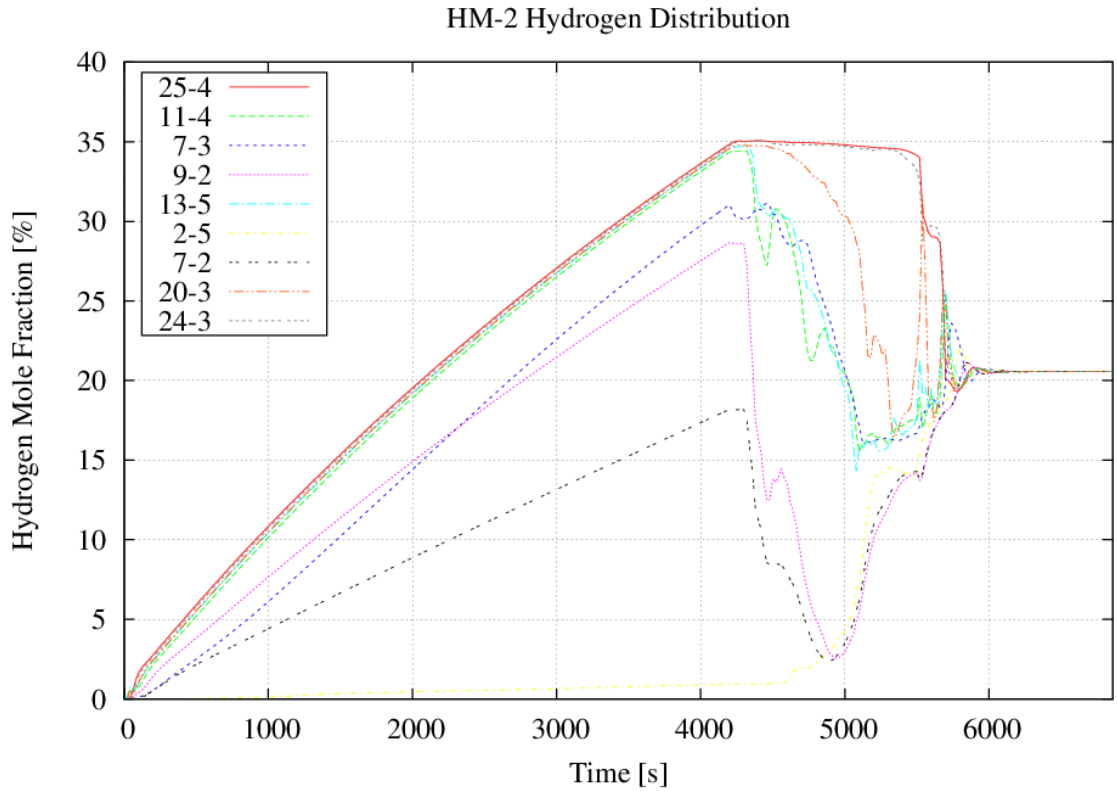


Figure 27. Hydrogen distribution calculated with APROS 6-equation model momentum transfer during injection

The results indicate that the momentum transfer has minor effect on the calculation results. This can be verified by examining the pressure head of the momentum convection term, which can be calculated as:

$$\Delta p = \rho u^2 \quad (12)$$

For example, by using $1.2 \frac{\text{kg}}{\text{m}^3}$ for density and $0.2 \frac{\text{m}}{\text{s}}$ for velocity, it is obtained 0.05 Pa for the pressure head, which is negligible.

In the experiment HM-2, the gas velocities are relatively slow that makes the pressure head of the momentum convection almost negligible. This is true under the conditions of the HM-2 experiment. But as was seen in the test case examined in Chapter 6.1.2, the momentum transfer may have an important effect on the pressure differences in other situations, where the source injection rate, and consequently, the gas velocities are very high.

6.4.4 Injection Zone

In the last simulation consideration examined before the comparison of experimental and calculated results, the effect of the injection zone nodalisation on the calculation results was studied. The minimum number of iteration cycles was nine and no momentum transfer was used. Figure 28 presents the calculated results of hydrogen distribution in the HM-2 experiment calculated with the APROS six-equation model.

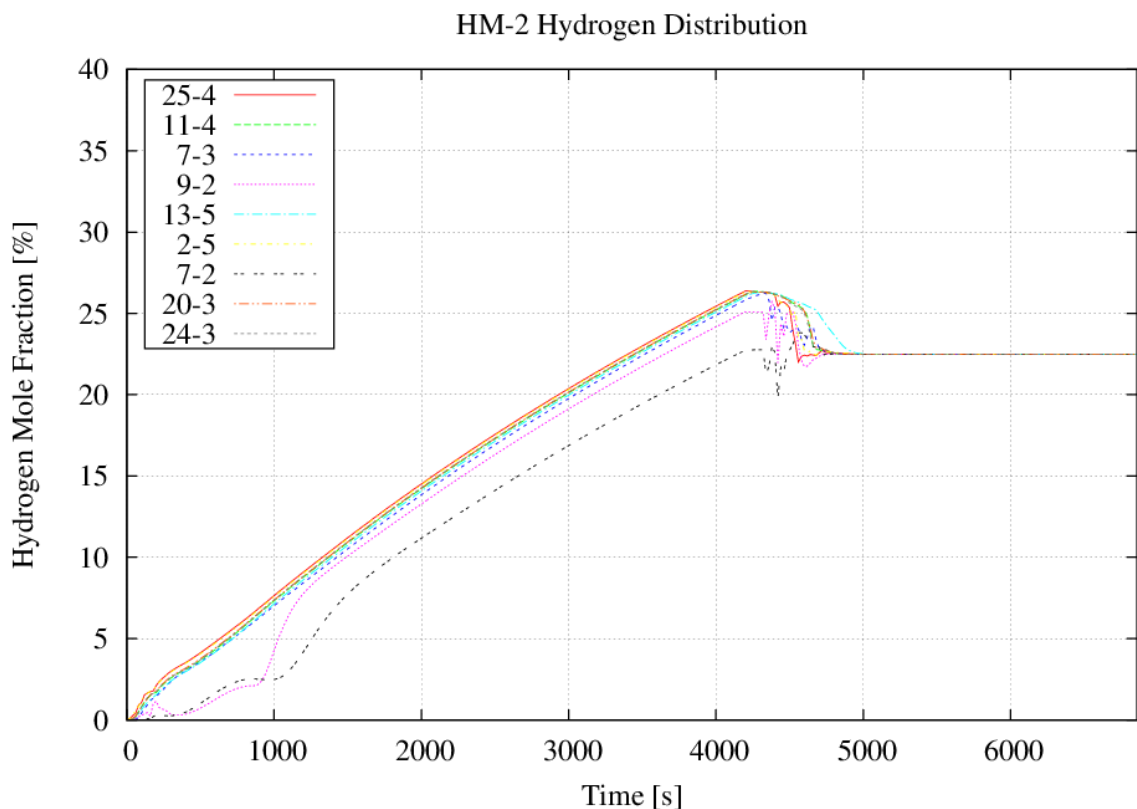


Figure 28. Hydrogen distribution calculated without the injection zone nodalisation

Without the injection zone nodalisation the hydrogen volume concentration raised to 26 % at the top of the vessel, which is considerably lower than the measured value of 37 %. And the overall stratification of the injected hydrogen was minimal. The calculation results confirm that in order to model the gas distribution with a LP code reliably, it is crucial to model additional flow paths which will describe the assumed flow paths of the injection plume or a jet.

6.5 Comparison of Experimental and Calculated Results

The HM-2 experiment can be divided into two phases. The first phase was the hydrogen injection phase (0 ... 4200 s) where hydrogen and steam were injected into the test vessel in a rate of $0.297 \frac{\text{g}}{\text{s}}$ with $0.243 \frac{\text{g}}{\text{s}}$, respectively. The injection phase lasts 4200 s and the atmosphere was let to stabilise for 120 s (stabilisation phase 4200 ... 4320 s), before the second phase (4320 ... 6820 s) of steam injection at a rate of $24.1 \frac{\text{g}}{\text{s}}$ is started. In the phase 1 the hydrogen was injected into the THAI facility at upper level of + 4.8 m and in the phase 2 the steam was injected at the lower level at + 1.8 m just below the inlet of the inner cylinder.

6.5.1 Pressure

The calculation pressure of the APROS containment model and the six-equation model using momentum transfer in the vertical branches between the special injection nodes only during the injections are presented in Figure 29. The results are also compared to the experimental data.

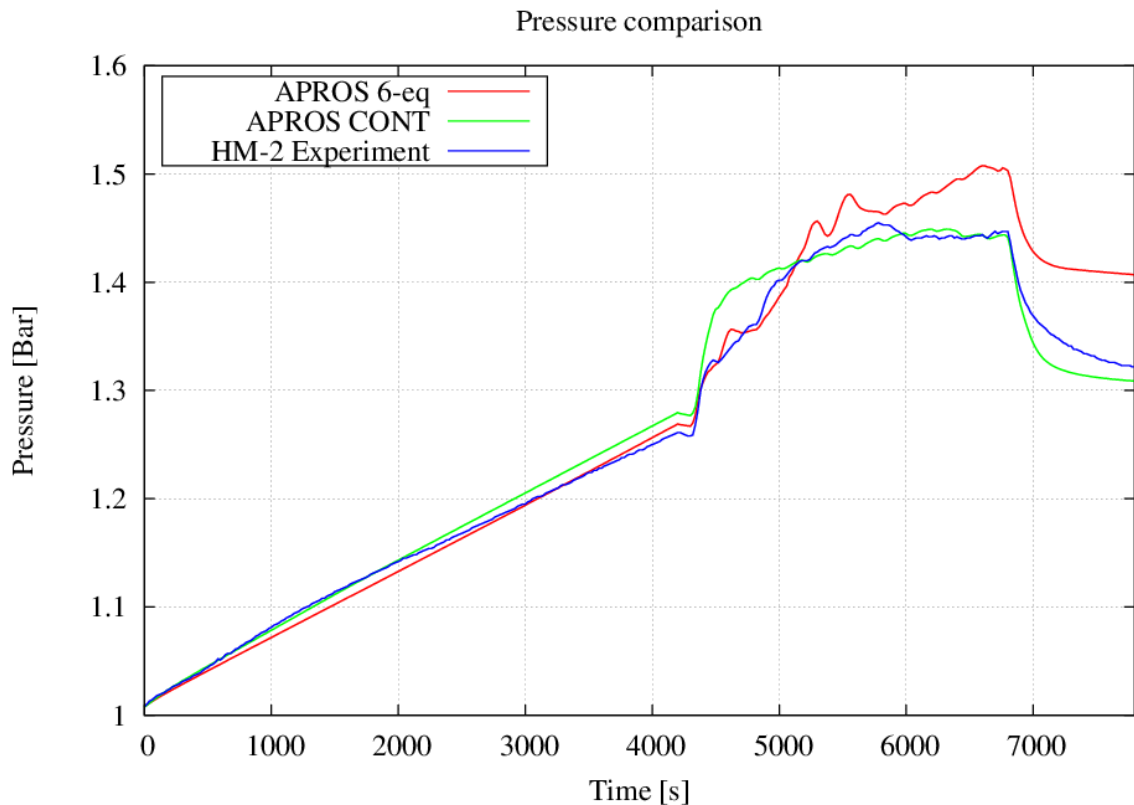


Figure 29. Calculated and measured pressures of HM-2 experiment

The atmospheric pressure is predicted extremely well by both the containment and the six-equation models until the end of phase 1. During the second steam injection phase some deviations are noticed. The APROS containment model predicts more rapid pressure increase immediately after the steam injection has started compared to the measurements and the results of the six-equation model. The reason for this is probably caused by the way steam condensation is modelled in the inner cylinder of the facility. It was observed during the simulations that the six-equation model calculated that the steam entering to the inner cylinder at the beginning of the injection was condensed very rapidly to the cold inner cylinder walls. But in the containment model the steam was condensed much slower.

During the second phase, the six-equation model predicts the pressure increase very well until 5100s of the experiment, but after that the pressure is over predicted to the end of the experiment. On the other hand, the containment model predicts the pressure almost consistently with the experiment from 5100 s to the end of the experiment. Generally speaking, both calculation models can predict the qualitative pressure history of the experiment very well.

6.5.2 Gas Temperatures

The gas temperatures in the top and bottom part of the vessel calculated with the APROS containment model and the six-equation model are presented in Figure 30. The results are also compared to the experimental data.

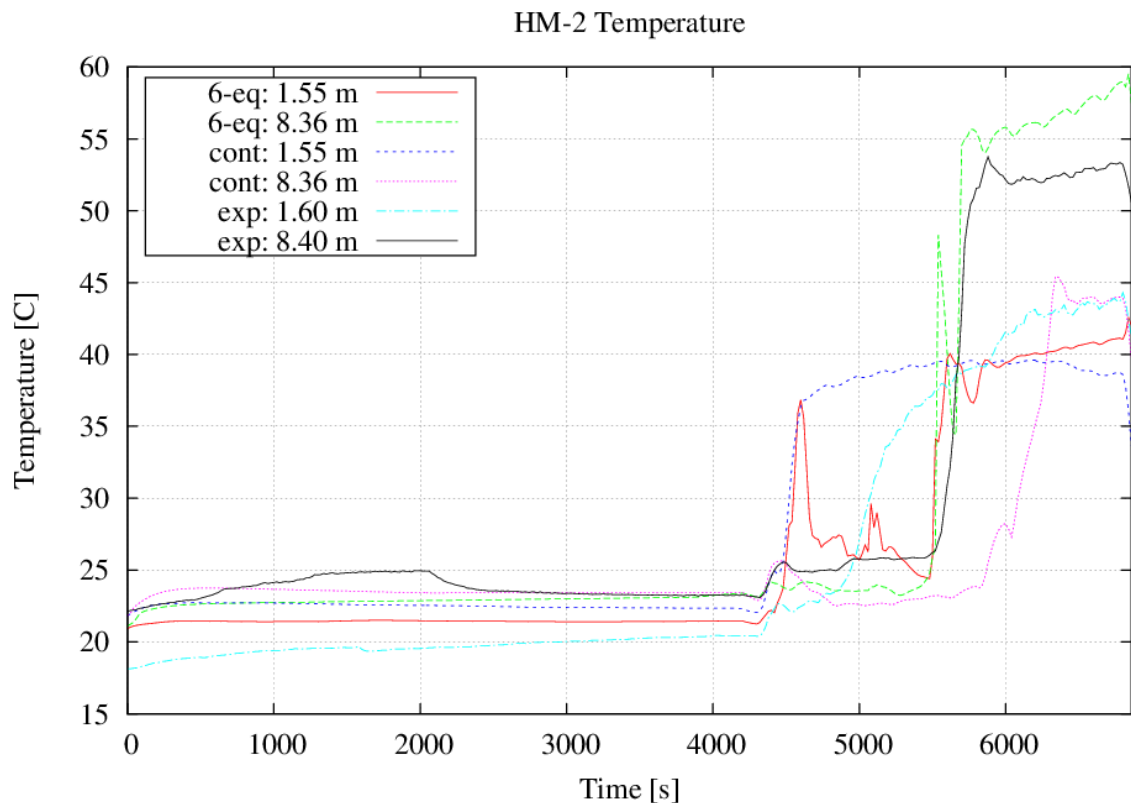


Figure 30. Calculated and measured gas temperatures at the top and bottom part of the THAI vessel

The measured temperature difference between the top and bottom part of the THAI facility is 4 °C at the beginning of the HM-2 experiment. In both calculations the temperature difference is only 1 °C, due to the initialisation of the calculation setup. There is almost no change in the temperatures during the hydrogen injection phase, and only slight temperature decrease is noticed during the stabilisation phase.

The gas temperatures are drastically changed during the steam injection phase. In the beginning of the steam injection the calculated gas temperatures in the bottom of the vessel start rising very rapidly. The six-equation model predicts that the gas temperature

in the annulus of the vessel at the level of the steam injections first rises very rapidly and afterwards decreases. This is probably caused by the fact that the code predicts that, in the beginning of the injection, some of the steam is flowing to the annulus area around the inner cylinder. The temperature in the annulus decreases because the majority of the injected steam is condensed in the inner cylinder, thus inducing flow that pushes the warm steam-gas mixture from the annulus to the inner cylinder. The containment model also predicts the temperature increase in the annulus, but not the similar kind of temperature decrease than observed with the six-equation model. This is probably caused by the fact that the containment model predicts the lower steam condensate rate in the inner cylinder than the six-equation model. The measured gas temperature in the bottom of the annulus of the vessel shows that the majority of the injected steam is entering directly to the inner cylinder, and the temperature inside the cylinder starts rising when the containment atmosphere starts to mix.

The six-equation model predicts the gas temperature at the top part of the vessel almost consistently with the experimental data. The containment model predicts that the temperature starts rising almost 300 s later than in the experiment and in the results of the six-equation model. It can be concluded that the containment model predicts that the atmosphere in the top part of the vessel is mixed later than in the experiment and later than predicted in the six-equation calculations.

6.5.3 Flow Patterns during Injections

The general qualitative flow patterns during the stratification and mixing phases is presented in the Figure 31.

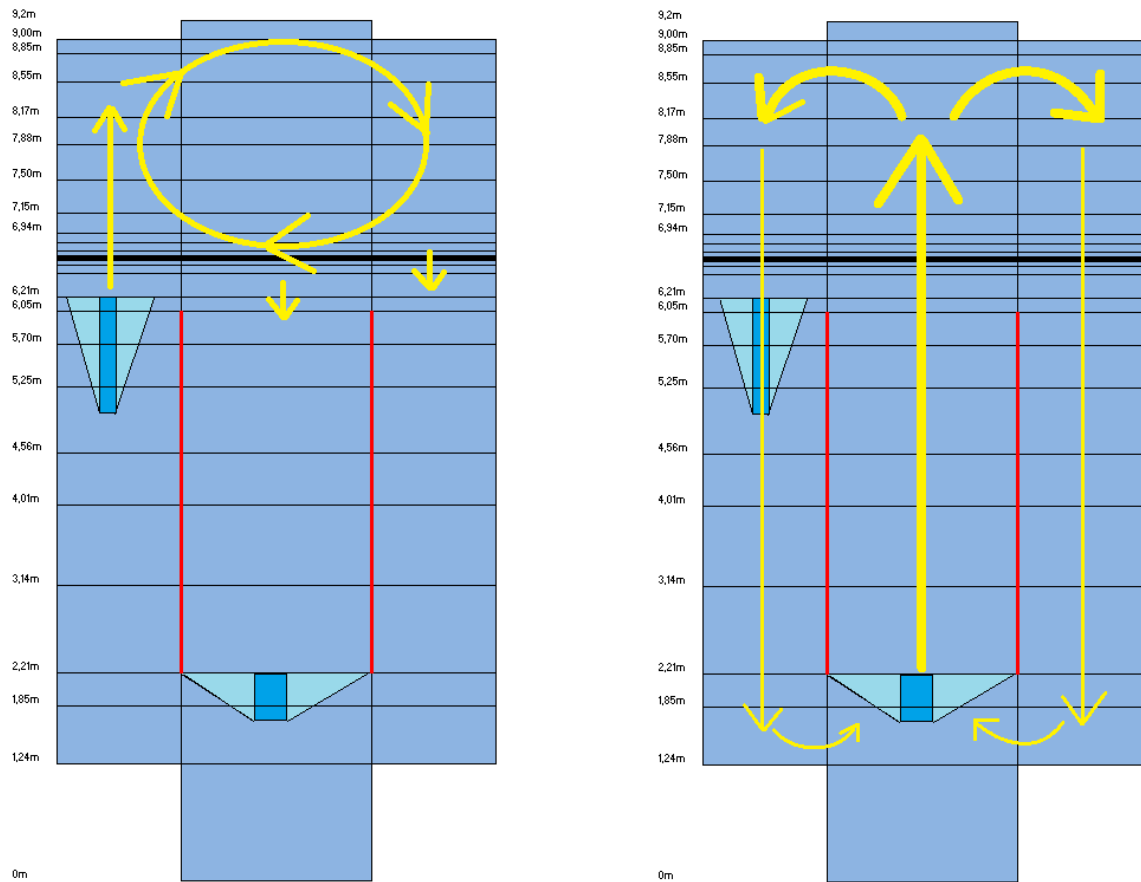


Figure 31. General flow patterns during the hydrogen and steam injections

There are three distinctly different flow phases during the HM-2 experiment. During the hydrogen injection phase the containment atmosphere is quite stable below the injection level (Figure 31, left side). As the hydrogen rises to the top of the test vessel a small natural circulation flow is induced in the top part of the vessel. Some amount of hydrogen is also flowing downwards inside and outside of the top part of the inner cylinder.

During the stagnation phase, in the beginning of the steam injection, the atmosphere of the vessel is mainly stabilised and no noticeable gas flows are present at the top and bottom and in the annulus of the vessel. Only noticeable flows are observed in the inner cylinder of the vessel.

During the mixing phase of the steam injection the steam flows through the inner cylinder and penetrates into the hydrogen-nitrogen cloud in the top of the vessel. Correspondingly, cooler gas mixture is flowing downward to the bottom part of the test

vessel through the annulus area of the vessel, thus creating a natural circulation flow in the entire vessel and, thus mixing the atmosphere.

6.5.4 Hydrogen Mole Fractions

During the first phase hydrogen coupled with steam tracer is injected into the vessel and a buoyant hydrogen-nitrogen plume rises up to the top of the vessel. At the end of the phase, a stable atmospheric stratification with hydrogen volume concentration of 37 % is established in the upper part of the vessel between level + 6.3 m and + 8.7 m. The hydrogen concentration below level + 3.1 m is very small, near 0 %. Between the upper and lower elevations a transition region was formed. (OECD – NEA 2010, 3.)

The measured and calculated hydrogen concentrations during the first injection and stabilisation phases are presented in the Figure 32, Figure 33 and Figure 34.

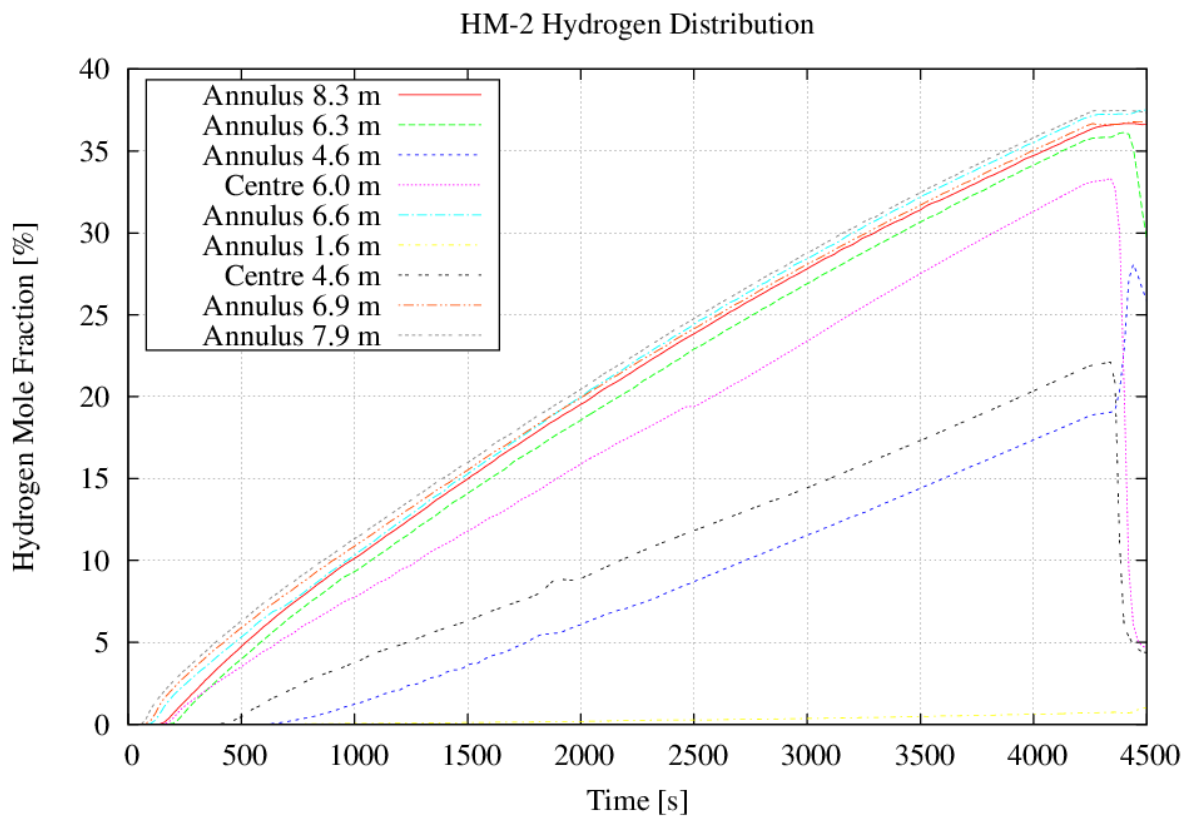


Figure 32. Measured hydrogen concentrations of the phase one of HM-2 experiment

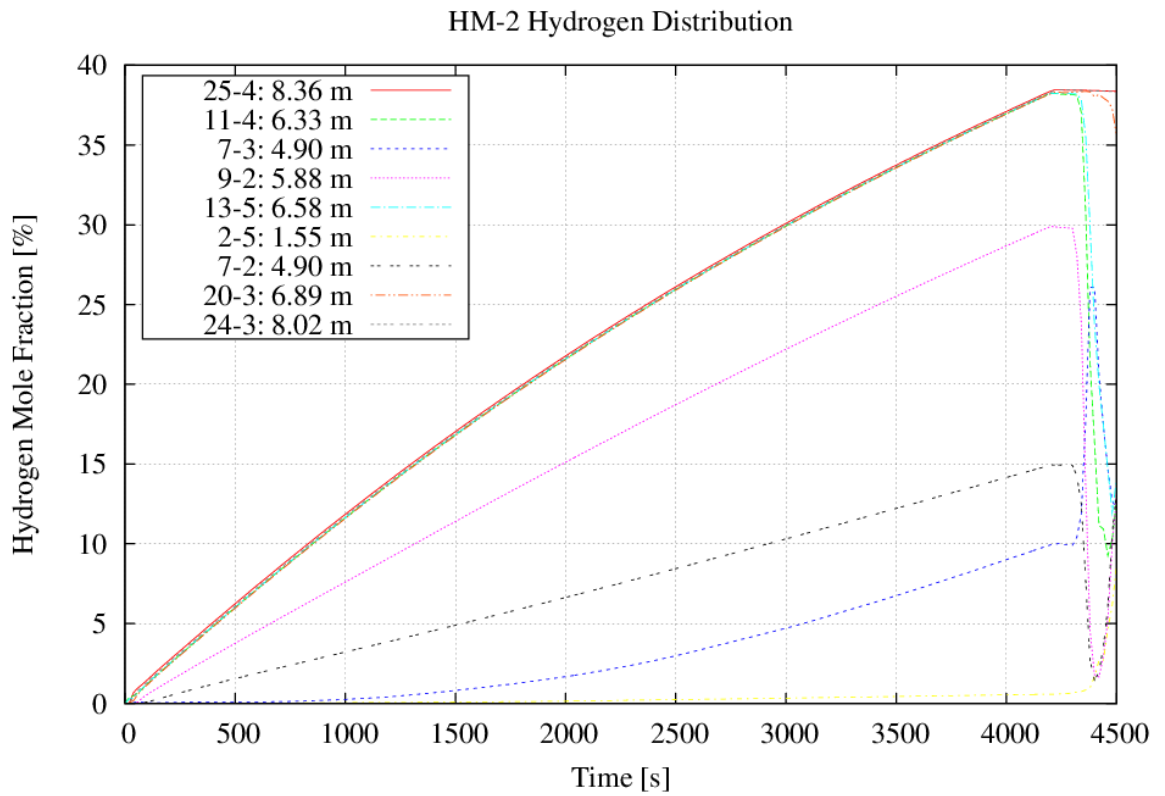


Figure 33. Hydrogen concentrations of the phase one of HM-2 experiment calculated with the APROS containment model

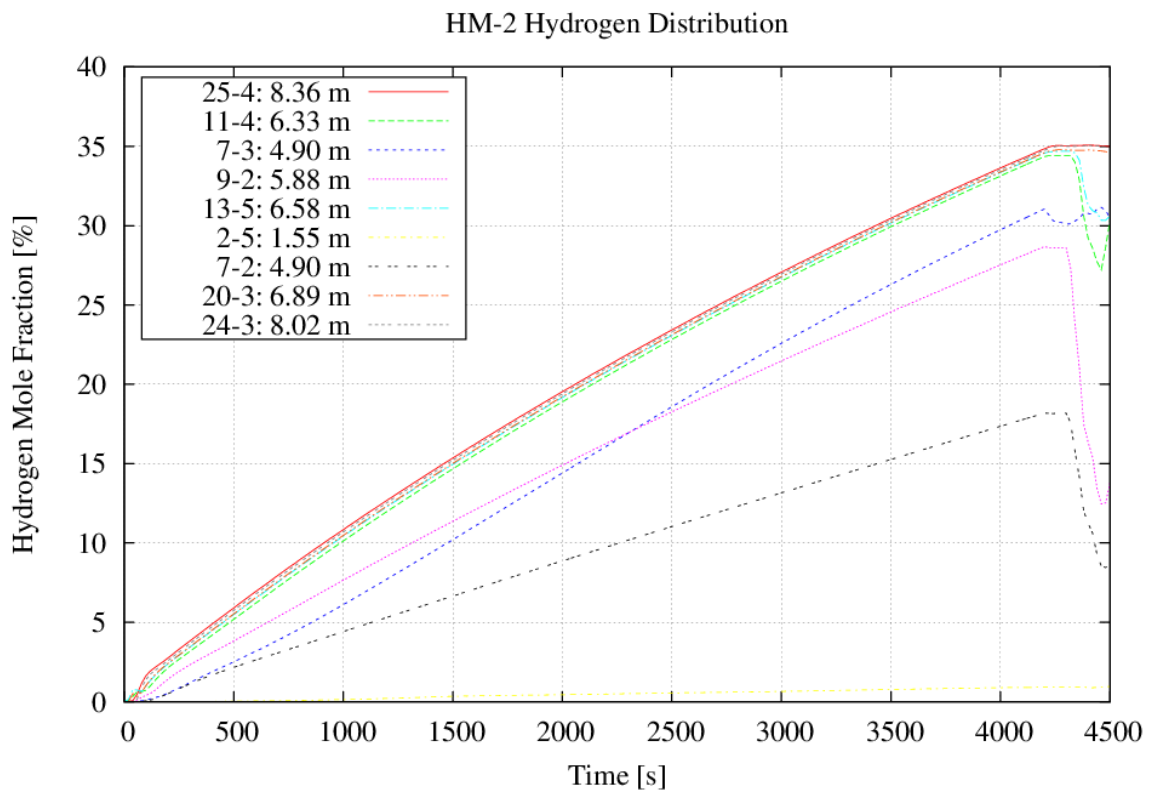


Figure 34. Hydrogen concentrations of the phase one of HM-2 experiment calculated with the APROS 6-equation model

The hydrogen stratification process is predicted relatively well by both models. Comparing to the measurements and the results of the containment model, the six-equation model predicts more hydrogen to be accumulated to the annular area of the THAI test vessel below the injection nozzle. The measured hydrogen volume concentration in the annular area of the vessel below the injection nozzle is 18 % in the end of the first phase, whereas the six-equation model and containment model predict 31 % and 10 % concentrations, respectively.

After the hydrogen has formed a stratified layer in the top part of the THAI facility, the second injection phase with steam is started. The injected steam enters the inner cylinder of THAI facility and a rising steam-nitrogen plume is formed in the cylinder. The steam injection phase can be divided into two sub-phases. During the so called stagnation phase the rising steam-nitrogen plume supersedes the hydrogen inside the inner cylinder. This phase lasts from the start of the steam injection at 4320 s to 4820 s. When the steam-nitrogen plume enters the hydrogen-rich layer in the top part of the vessel, a natural circulation flow is created and started at 4820 s. This is called a gas mixing phase. In the mixing phase, gas is rising in the inner cylinder and simultaneously hydrogen-rich gas flows downwards in the annulus mixing the atmosphere. The rising plume coming from the inner cylinder dissolves the hydrogen-rich cloud in the top vessel starting from the bottom of the cloud as detected from the Figure 35. (OECD – NEA 2010, 3.)

The measured and calculated hydrogen concentrations during the second injection phase of the HM-2 experiment are presented in the Figure 35, Figure 36 and Figure 37.

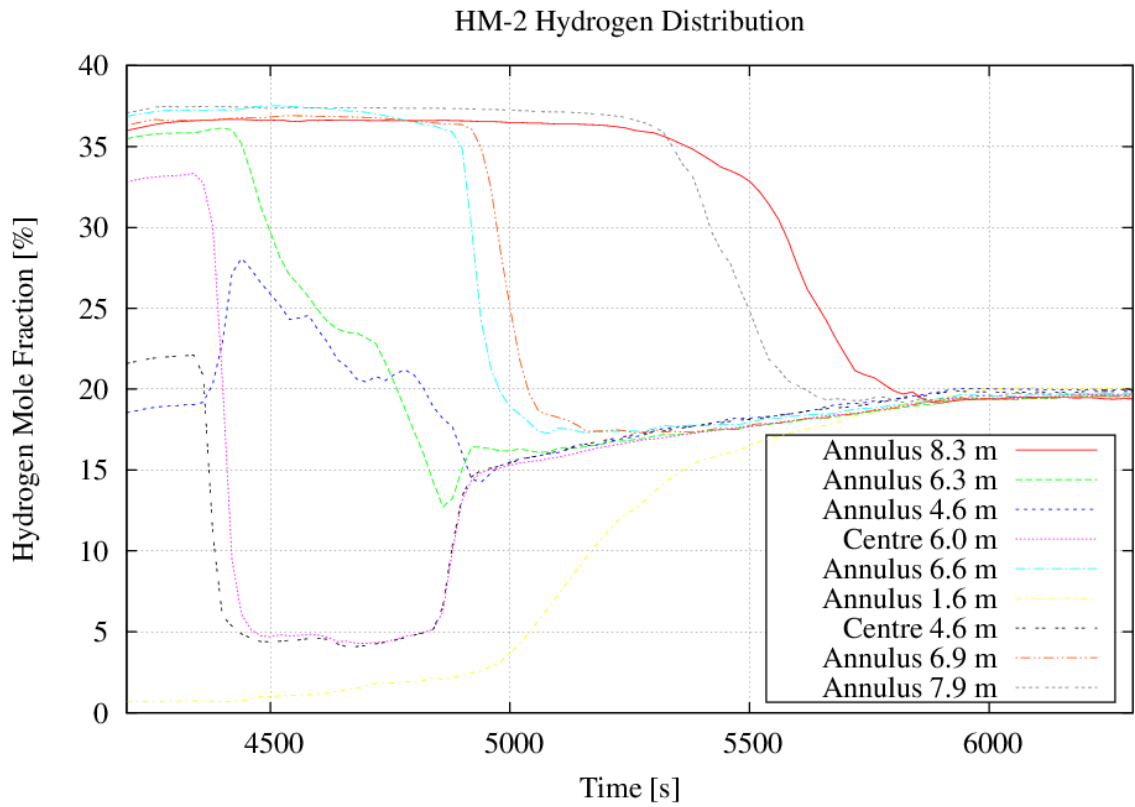


Figure 35. Measured hydrogen concentrations during the steam injection phase of HM-2 experiment

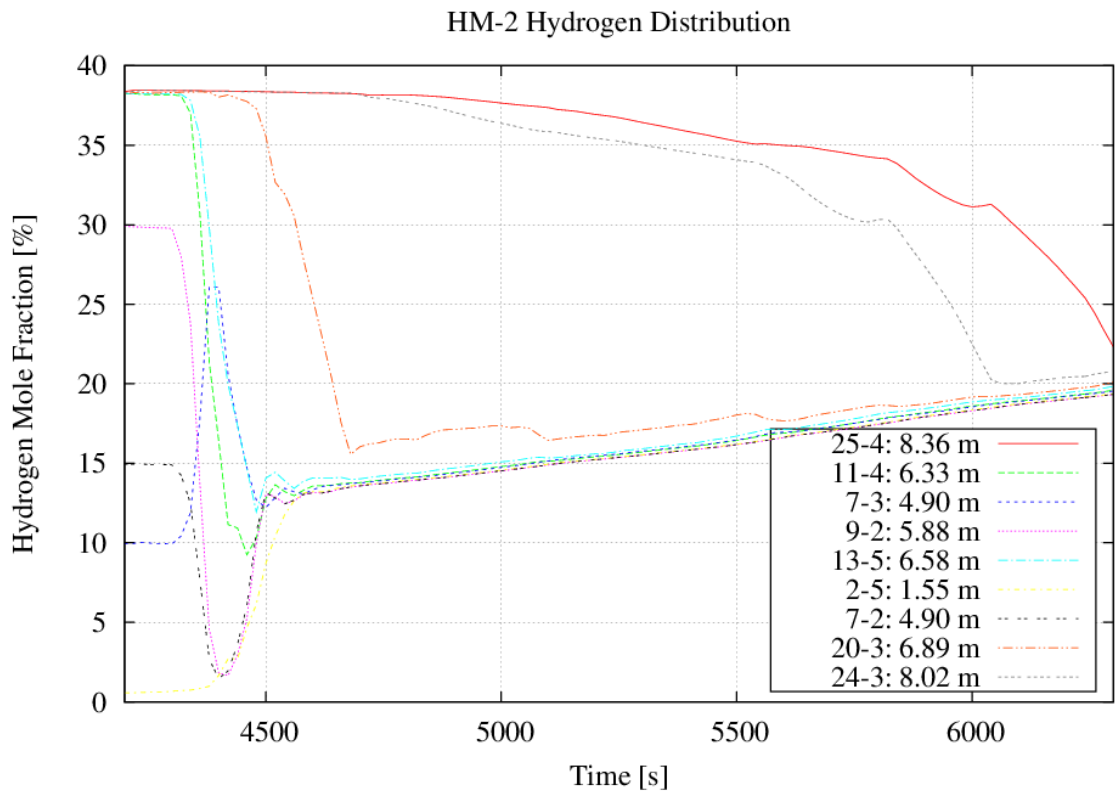


Figure 36. Hydrogen concentrations during the steam injection phase of HM-2 experiment calculated with the containment model

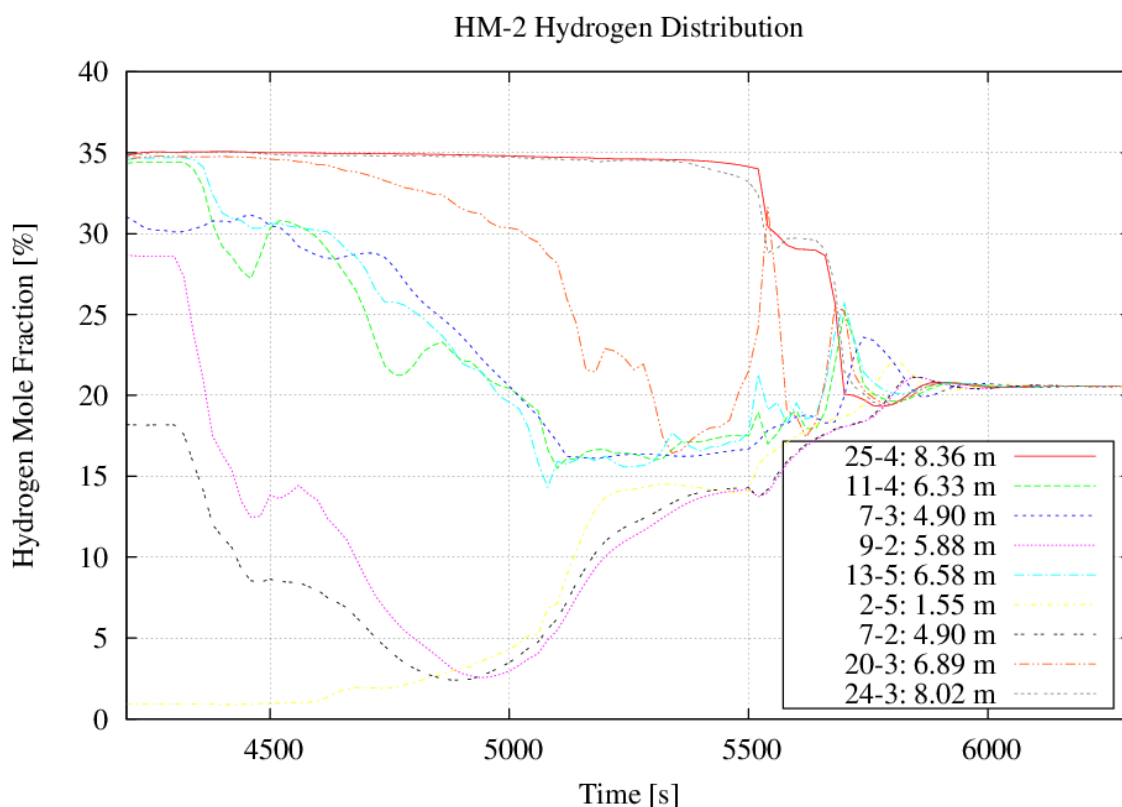


Figure 37. Hydrogen concentrations during the steam injection phase of HM-2 experiment calculated with the six-equation model

Both APROS models can predict better the build-up of the stratification than the dissolution of the stratified hydrogen cloud. The main reason for this is the need to resolve the stratified layer/plume interface region. Both calculation models can predict the stagnation phase and the onset of the natural circulation and gas mixing phase reasonably. The containment model predicts that the stagnation phase lasts from 4320 s to 4500 s. The six-equation model predicts that the stagnation phase lasts from 4320 s to 5100 s.

The measurements show that the atmosphere of the THAI facility was completely mixed around at 5900 s. The six-equation model predicts that the atmosphere is completely mixed at 5700 s and the containment model predicts that the dissolution process of the stratified layer lasts longer and the atmosphere is mixed later at 6400 s.

The measured and calculated vertical hydrogen distribution during the whole experiment is shown in the Figure 38, Figure 39 and Figure 40.

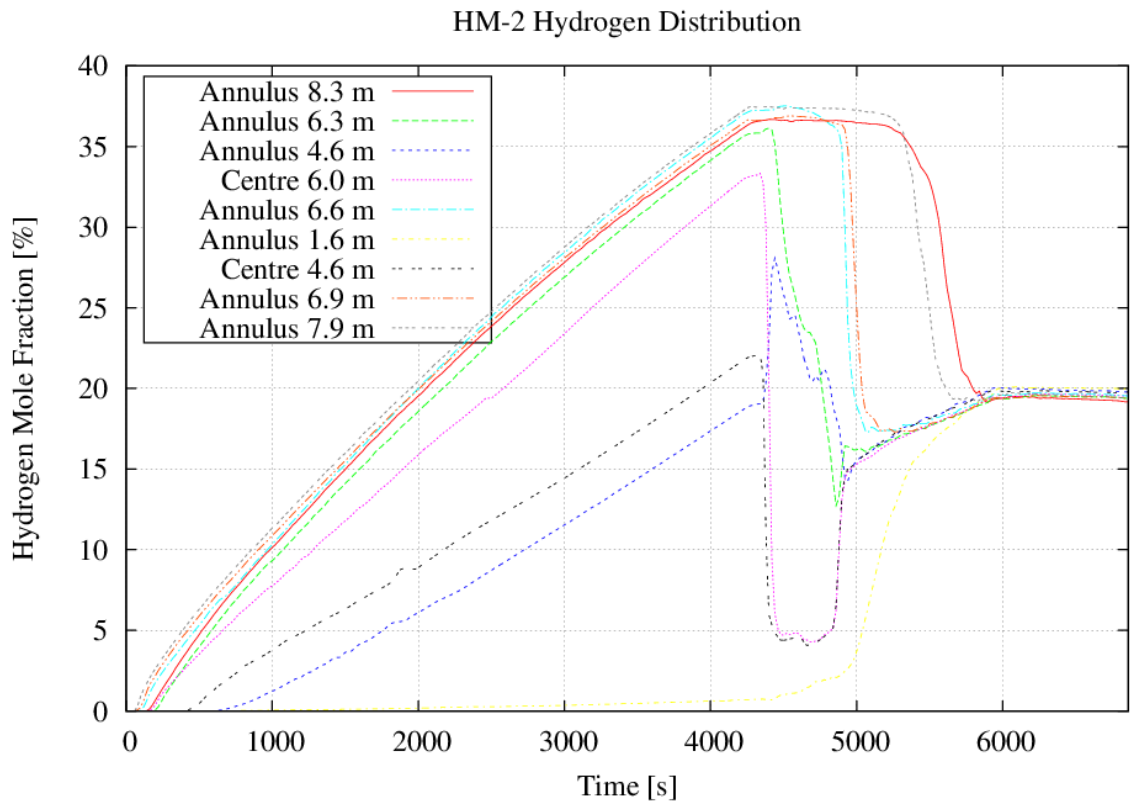


Figure 38. Measurement hydrogen distribution during the whole HM-2 experiment

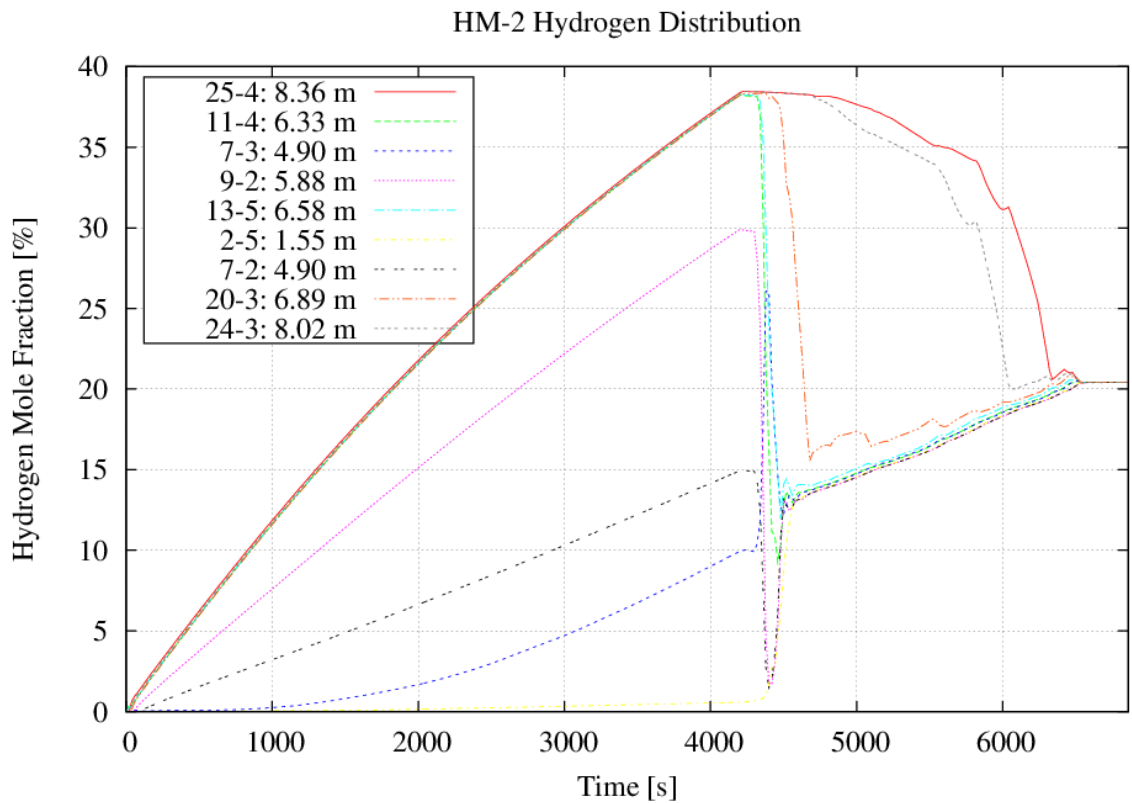


Figure 39. Calculated hydrogen distribution of the HM-2 experiment using the APROS containment model (whole experiment)

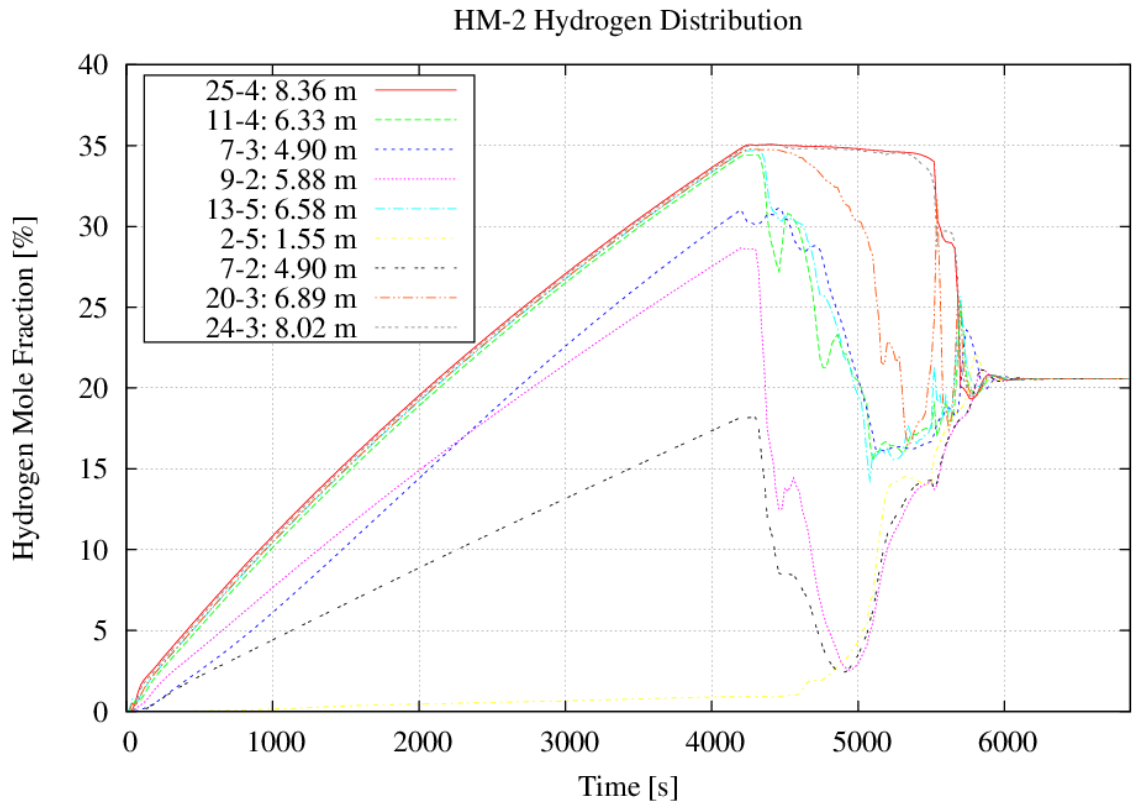


Figure 40. Calculated hydrogen distribution of the HM-2 experiment using the APROS 6-equation model (whole experiment)

In Figure 38, Figure 39 and Figure 40 it can be noticed that the APROS containment model and the six-equation model can qualitatively predict the formation and dissolution of a light gas cloud in the HM-2 experiment conducted in the THAI facility. The hydrogen injection phase of the HM-2 experiment was predicted by both codes almost consistently. Some discrepancies are noticed between the measured and calculation results during the stratification break up phase of the experiment. The six-equation model predicts that the stratification brake-up occurs 200 s faster than in the experiment. On the contrary, the containment model predicts that the stratification break up lasts 700 s longer than in the experiment. The calculation results verify that the both models have an ability to calculate the hydrogen stratification and gas mixing phenomena reasonably well.

7 CONCLUSIONS

In this master's thesis hydrogen stratification and atmosphere mixing modelling with LP codes was studied. The hydrogen stratification and dissolution experiment HM-2 conducted at the THAI test facility was calculated using the APROS LP containment model and the six-equation model. In the simulations, identical sub-compartment nodalisation was used that included special nodalisation for the injection zones. The experiment was simulated with the APROS six-equation model with different calculation options to gain better understanding on the capabilities of the calculation model to containment applications.

The calculation results showed that both the APROS containment and the 6-equation model were able to model the hydrogen stratification in the THAI test well, if the limitations of the codes are taken in consideration in the preparation of the input deck. Also the vertical distribution of containment nodalisation should be detailed enough. The more vertical levels the nodalisation has, the more accurate are the calculation results. Special nodalisation for the injection zone is also needed to simulate the effect of a plume or a jet gas flow satisfactory. The APROS six-equation model is able to predict atmosphere stratification and mixing in situations with high concentrations of non-condensable gases and slow flows accurately, if the minimum number of iterations is set high enough. It was concluded that using at least nine or more iteration cycles, the mass error becomes small enough to get reasonable and accurate results.

Modelling of the dissolution process of the stratified hydrogen cloud proved to be more challenging task. Nodalisation of the calculation models used was designed to be in line with the measurement instrumentation of the THAI facility. The calculation results of the HM-2 experiment could possibly be improved by making denser vertical nodalisation of the THAI test vessel above the upper outlet of the inner cylinder. In the present THAI nodalisation, the inner cylinder volume is modelled with one nodalisation stack so flow that occurs simultaneously to two different directions inside the cylinder cannot be modelled. If the inner cylinder volume would be modelled with two node stack, the other being central volume and the other annulus volume adjacent to the cylinder wall, it could improve the simulation results.

The one objective of this thesis was to determine, whether it would be useful to add the convection term in the momentum conservation equation of the APROS containment model. The evaluation was done by calculating a containment test cases and the HM-2 experiment with the APROS six-equation model (with and without the momentum transfer option) and the APROS containment model. The results obtained from the HM-2 test, where the flow velocities were low (less than 1 m/s) suggested that the effect of the momentum transfer option is almost negligible. On the other hand, the results from the containment loading test case showed that the momentum transfer has influence on the pressure differences between the adjacent nodes, if the gas velocities inside the containment were very high, in this test case almost 300 m/s, which resulted also in high values for the momentum convection terms. From these two simulation cases it can be concluded that the momentum transfer may have an effect to the results in the containment applications. If the gas flow rates are relatively low, the convection term of the momentum conservation is insignificant. On the other hand, if gas velocities are very high, the momentum transfer may have influence on the predicted pressure differences between the adjacent nodes. It could also be really beneficial for the evaluation process of determining the importance of the momentum transfer, if a well instrumented separate effect experiment involving plume and jet gas flow test was calculated and analysed.

Despite both the APROS LP containment and six-equation models could calculate the hydrogen stratification well in case of the THAI test under consideration, in more complicated cases; the numerical diffusion may distort the results. Calculation of light gas stratification could be probably improved by applying the second order discretisation scheme for modelling of gas flows.

In addition to the default correlations and other simulation options in APROS there are a lot of possibilities to control the simulations. Therefore, good user guidelines are needed for code users to perform reliable calculations. These guidelines should include every aspect of the simulation starting from the preparation of the nodalisation to the computational settings of the simulation. These include choosing the appropriate calculation correlations and other user input options included in the program.

8 SUMMARY

Hydrogen stratification and atmosphere mixing is a very important phenomenon in nuclear reactor containments when severe accidents are studied and simulated. Hydrogen generation, distribution and accumulation in certain parts of containment may pose a great risk to pressure increase induced by hydrogen combustion, and thus, challenge the integrity of NPP containment. The accurate prediction of hydrogen distribution is important with respect to the safety design of a NPP.

Modelling methods typically used for containment analyses include both lumped parameter and field codes. The lumped parameter method is universally used in the containment codes, because its versatility, flexibility and simplicity. The lumped parameter method allows fast, full-scale simulations, where different containment geometries with relevant engineering safety features can be modelled. Lumped parameter gas stratification and mixing modelling methods are presented and discussed in this master's thesis

The HM-2 experiment related to hydrogen stratification and mixing conducted at the THAI facility in Germany is calculated with the APROS lump parameter containment package and the APROS 6-equation thermal hydraulic model. The main purpose was to study, whether the convection term included in the momentum conservation equation of the 6-equation modelling gives some remarkable advantages compared to the simplified lumped parameter approach. Finally, a simple containment test case (high steam release to a narrow steam generator room inside a large dry containment) was calculated with both APROS models. In this case, the aim was to determine the extreme containment conditions, where the effect of convection term was supposed to be possibly high. Calculation results showed that both the APROS containment and the 6-equation model could model the hydrogen stratification in the THAI test well, if the vertical nodalisation was dense enough. However, in more complicated cases, the numerical diffusion may distort the results. Calculation of light gas stratification could be probably improved by applying the second order discretisation scheme for the modelling of gas flows. If the gas flows are relatively high, the convection term of the momentum

equation is necessary to model the pressure differences between the adjacent nodes reasonably.

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