# Modeling of the QUENCH-14 bundle experiment using ASTECv2.0R2p2 

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## Introduction

- The QUENCH experiments investigate the $\mathrm{H}_{2}$ source term resulting from the water injection into an uncovered core of LWR as well as the high temperature behavior of core materials under transient conditions
- The aim is to present the results of the QUENCH-14 modeling by the ASTEC code to trhe CESAM community. Both Techn. Univ. Sofia and KIT are adopting the ASTEC code for modeling several QUENCH experiments.


## The QUENCH-14 experiment

In the QUENCH-14 experiment, the effect of $\mathbf{M}{ }^{\ominus}$ cladding material on bundle oxidation and core reflooding was investigated, in addition to the former QUENCH-06 test that used Zry-4. The bundle configuration of QUENCH-14 with 1 unheated rod, 20 heated rods, and 4 corner rods was identical to the design of QUENCH-06.

The QUENCH-14 test was conducted in principle with the same protocol as QUENCH-06, so that the effects of the change of cladding material could be observed more easily ( a "one-parameter" investigation).
QUENCH-6 was already modeled using ICARE/CATHARE in the frame of the ISP-45 (Benchmark Exercise)

## QUENCH-14 facility



The test section is enclosed by a safety containment. Superheated steam from the SG and super heater together with Ar enter test bundle at the bottom. Ar, steam and $\mathrm{H}_{2}$ produced in the $\mathrm{Zr}-\mathrm{H}_{2} \mathrm{O}(\mathrm{g})$ reaction flow upwards inside the bundle and from the outlet at the top through a water-cooled off-gas pipe to the condenser, where the remaining steam is separated from the noncondensable gases Ar and $\mathrm{H}_{2}$.

# QUENCH-6/-14 bundle 



Fuel rod simulator

The test bundle is made up of 21 fuel rod simulators and of 4 corner rods. The fuel rod simulators are held in their positions by 5 grid spacers, 4 of Zry-4, and one of Inconel 718 in the lower bundle zone.
The rod cladding of the heated and unheated fuel rod simulator is $\mathrm{M} 5^{\circledR}$ (product of AREVA)
The max. total power during the $\mathrm{Q}-14$ test was 19 kW . About $40 \%$ of it being released into the inner rod circuit (8 fuel rod simulators); $60 \%$ in the outer one ( 12 fuel rod simulators).
The test bundle is surrounded by a 3.25 mm thick shroud ( 80 mm ID) made of Zry-4 with a 37 mm thick ZrO 2 fiber insulation and an annular cooling jacket made of Inconel 600 (inner tube) and SS (outer tube).

## QUENCH-14 test phases



Heatup to ~873 K. Facility check.
Phase I Stabilization at $\sim 873 \mathrm{~K}$.
Phase II Heat-up with $\sim 0.3-0.6 \mathrm{~K} / \mathrm{s}$ until $\sim 1500 \mathrm{~K}$ is reached.
Phase III Pre-ox of the bundle in a mix flow of $3 \mathrm{~g} / \mathrm{s}$ of $\mathrm{H}_{2} \mathrm{O}_{(\mathrm{g})}$ superheated to 783 K \& $3 \mathrm{~g} / \mathrm{s}$ Ar for $\sim 3000 \mathrm{~s}$; peak temp. of $\sim 1500 \mathrm{~K}=$ const. Withdrawal of the corner rod B at the end of that Phase.
Phase IV Transient heat-up with 0.3... $2.0 \mathrm{~K} / \mathrm{s}$ from $\sim 1500$ to $\sim 2050 \mathrm{~K}$ in the same flow conditions. Withdrawal of the corner rod D ~30 s before quench starts.
Phase V Quenching of the test bundle using a high flow of $\sim 41 \mathrm{~g} / \mathrm{s}$ of $\mathrm{H}_{2} \mathrm{O}_{(I)}$.

# WASTEC input deck (ID) adaptation for QUENCH-14 

The existing QUENCH-05 ID was used, developed by S. Melis (IRSN), slightly optimized by W. Hering for ASTECv1.3R2 \& adapted as Q-06 by H. Muscher (both KIT).

QUENCH-06 ID changes towards the ASTECv2.0R2p2 / ICARE requirements have been made by P. Kaleychev; the changes in style/ syntax were the following:

- The module itself was adapted from 'DIVA' to 'ICARE'. All the structures with the name 'DIVA' were renamed to 'ICARE'
- Everywhere in the ID, the descriptor 'VESSEL_D' was changed to 'VESSEL'
- In the structure 'STRU CONNECTI', the TYPE 'SOURCE' was changed to 'BREAK', according to a recommendation of $S$. Bertusi (IRSN)- answer to a MARCUS card call.
- Structure for modeling of the fluid convection was subdivided into two structures, as every of the two structures contains only one fluid channel: CAN1 and WCAN1
- Suppressing of the option 'CONT 0' for imposed contact of the shroud was done to obtain better visualization of the color coded shroud temp. field - hint of S. Bertusi, too.


## Further QUENCH-14 ID tuning

To change the QUENCH-06 ID according to the exp. conditions of QUENCH-14:

- For the temp. range (1073-1673) K, the M5 ${ }^{\ominus}$ oxidation kinetics data proposed after the SET measurements at KIT (M. Große) were taken. For the temp. range (1674-2050) K the existing data for Zry -4 were used instead that of $\mathrm{M} 5^{\circ}$ since the needed $-\mathrm{M} 5^{\circ}$ values are not available
- El. power histories for both sub circuits of heated rods were changed in accordance to Q-14 experimental results.
- Visualization: 3 figures were additionally produced: the $\mathrm{H}_{2}$ rate $[\mathrm{kg} / \mathrm{s}]$, the layer thickness evolution of the cladding [ $\mu \mathrm{m}$ ] vs. time and the cladding layer thicknesses [ $\mu \mathrm{m}$ ] for given rod elevation / according ASTEC structures were developed by S. Bertusi

By all these implementations, changes/ improvements in the QUENCH-14 IDs -both for ASTECv2.0R2p2 and ASTECv1.3R2 several runs were performed, allowing a comparison of the results given by the older and newer ASTEC-versions, respectively.

## Results using ASTECv2.0R2p2



Temp. histories - experimental data


According temperatures - ASTECv2.0R2p2

Calculated max. temp. (right side) is close to the exp. Q-14 data at "hottest" elevation of 950 mm (left), the but max. calculated value just before quenching is ca 2000 K in comparison to 2150 K for the exp. This lower max-value may be explained with the ox correlation for Zry-4 used for the highest temp-s.

## Results of ASTECv2.0R2p2: temp. histories

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Rod temp. - heat-up phase


Rod temp. - transient \& quench phases from the inner ring ( 8 rods) (TFS4/9) and for one heated rod from the outer ring of 12 rods (TSH5/0).
The highest temp.-s were calculated for the inner rod TCRC13, where the max. value of about 1900 K is found just before quench. For the same time the temp. of TFS4/9 is about 1500 K ; the temp. of rod TSH5/0 is 900 K . There is an acceptable difference of about 100 K for all of the three rods in comparison to the exp. Q-14 data.

# ASTECv2.0R2p2-results: some axial temp. profiles 

 Axial temp profiles -start of the pre-ox
phase, 3000 s Axial temp profiles -start of the pre-ox
phase, 3000 s
Axial temp. profiles on the end of reflood, 7300 s , beginning of quenching


The axial temp. profiles from the beginning till the quench phase are similar for the heated rod, the shroud, the unheated and the corner rod. They are higher in comparison to the temp. of the cooling jacket. The highest temp. is calculated for the heated rod in the height of about 950 mm , exactly as it was in the $\mathrm{Q}-14$ experiment.

After the beginning of the quench phase, the temp.-s of the heated, unheated and the corner rods as well as that of the shroud start to decrease (here $\tau=7300 \mathrm{~s}$ ) in correspondence to the rapid increase of the quench water level. In the end of the calc., the highest temp.-s at levels down to 1 m were calculated over the cooling jacket with a max. detected at a height ca. 750 mm ( $\tau=7600 \mathrm{~s}$ ). At heights up to 1 m the temp.-s of the heated rod, shroud, the unheated and the corner rod remain higher in comparison to the temp. of the cooling jacket.

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## Results of ASTECv2.0R2p2: nodalization



ASTEC- temp. field in the beginning of pre-ox phase (3000 s)


Temp field at the end of experiment (7600 s)

The temp. fields for the central rod (U), one of the heated rods from inner ring (H1), one heated rod from the outer ring (H2), two corner rods (C1 and C2), shroud and insulation. The highest temp. before quenching are calculated for height of ca. 950 mm . In the end of the calculation (at 7600 s ) the highest temp. are calculated over the insulation at height around 750 mm and above.

## Results of ASTECv2.0R2p2: oxide layer



Oxide thickness profile, 7600 s , unheated rod - ASTEC


Oxide thickness profile, 7600 s, inner ring rod - ASTEC


Oxide thickness profile, 7600 s , Shroud - ASTEC

The max. oxide thickness calc. by ASTEC for the central unheated rod (Fig. left, CLAD1), is ca. $630 \mu \mathrm{~m}$ at a height around 950 mm in comparison to $860 \mu \mathrm{~m}$ at the same height from the $\mathrm{Q}-14$ exp. At the same height, approx. equal (around $650 \mu \mathrm{~m}$ ) is the max. layer thickness for inner ring rod (CLAD2). For the rod from the outer ring, the max. oxide thickness is about $630 \mu \mathrm{~m}$ at the height of ca. round 950 mm . In the shroud (BZIR) the calculated oxide thickness is of ca $650 \mu \mathrm{~m}$ : is similar to the exp. value of $590 \mu \mathrm{~m}$. In all the fig-s depletion of the metal- layers is visualized (abs. value being equal to the oxide thicknesses)

## ASTECv2.0R2p2 results: formation of $\alpha-\mathrm{Zr}(\mathrm{O})$ and $\mathrm{ZrO}_{2}$ cladding layers



Cladding layer thickness evolution, 950 mm, unheated rod - ASTEC


Cladding layer thickness evolution, 950 mm , inner ring rod - ASTEC


Cladding layer thickness evolution, 950 mm , outer ring rod - ASTEC

According to the height of max. calculated oxide thickness, which was at 950 mm , the cladding layer thickness evolution for the whole time of the Q-14 exp. was modeled. In the end of calc. the fraction ratio of $\alpha-\mathrm{Zr}(\mathrm{O})$ becomes the largest one for all the 3 cases - unheated rod, inner ring and outer ring rod, on the second place - the fraction of $\mathrm{ZrO}_{2}$ and in the end - the Zr contribution. In the case of inner ring rod oxidation one can postulate that the according oxide thicknesses ( $\alpha-\mathrm{Zr}(\mathrm{O})$ and $\mathrm{ZrO}_{2}$ ) are only a little bit larger than in the cases of the unheated rod (left) and outer ring rod oxidation (right).

## Results of ASTECv2.0R2p2: hydrogen release


$\mathrm{H}_{2}$ prod. - Q-14 exp. data vs. an ASTEC -line

The calculated $\mathrm{H}_{2}$ production by ASTECv2.0R2p2 is about 32 g ( 40 g in the $\mathrm{Q}-14$ experiment).
The results obtained by ASTEC are close to the exp. data in the phases before quench. Because at the high temp.-s range (1674-2050) K data of Zry-4 instead of M5 were used (mentioned two times above), the obtained results for $\mathrm{H}_{2}$ prod. at quench itself are under-estimated.
Discussion of other possible reasons for that: - up till now no modeling of important phenomena like

1) $\mathrm{H}_{2}$ abs. \& release by the cladding material,
2) Melt oxidation in-between cladding \& pellets;
3) formation of a quite thick (non-uniform?) oxide layer at the inner cladding surface in the region of melt formation.

# \【TComparison of ASTECv2.OR2p2 and ASTECv1.3R2 <br> Karlsruhe Institute of Technology 



Q-14: $\mathrm{H}_{2}$ production
exp. data vs. ASTECv2.0R2p2 modeling


Q-14: $\mathrm{H}_{2}$ production
exp. data vs. modeling with the old ASTECv1.3 version

In the case of ASTECv1.3R2 for the $\mathrm{Q}-14$ calc. (Fig. left) the obtained $\mathrm{H}_{2}$ masses are overestimated in the pre-ox phase and underestimated in the quench phase by the same reason as in the case of the ASTECv2.0R2p2 calc. mentioned above. The calc. integral $\mathrm{H}_{2}$ prod. Given by ASTECv1.3-35 g in comparison to the 40 g coming directly from the experiment.

## Conclusions

- The adapted ASTEC input decks for QUENCH-14 led to calculation results which are similar to experimental data. This is encouraging for our future CESAM activities. The newest version of the ASTECv2.1 code (still under development) will surely give us a further chance for even more accurate modeling of the Quench-phenomena.
- Concerning our QUENCH-14 approach: after getting some technical assistance from IRSN, the following important aspects of the QUENCH-14 process were modeled quite correct:
- 1) the position of the hottest zone in the test bundle,
- 2) the generation of $\mathrm{H}_{2}$ in the different phases of the experiment,
- 3) the thicknesses of the oxide layers both over time and height of the rod bundle .

In our ASTEC modeling only the part of outer cladding oxide has been incorporated. Apart of the fact that, the post-test metallographic inspection after the Q-14 experiment showed relative thick inner oxide layers in the claddings (up to $150 \mu \mathrm{~m}$ ) above the elevation of ca. 950 mm , too.
Although some little differences in the validation of the $\mathrm{Q}-14$ modeling results towards experiment exist (especially for the QUENCH phase itself) one can be optimistic looking for the next stage- i.e. the QUENCH-10 \& especially QUENCH-16 modeling.

