KIT Validation Activities of the ASTEC code against the QUENCH Bundle Experiments: Results and Outlook

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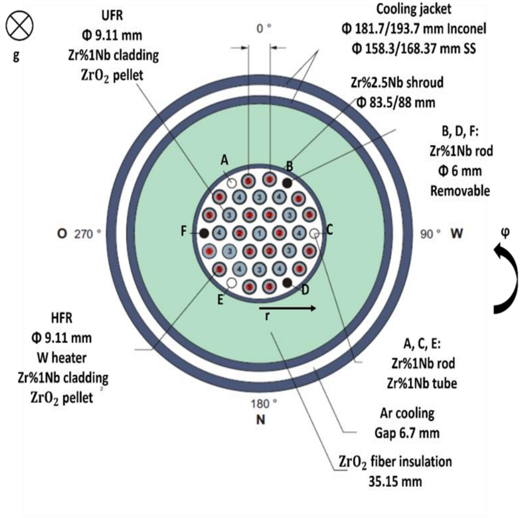
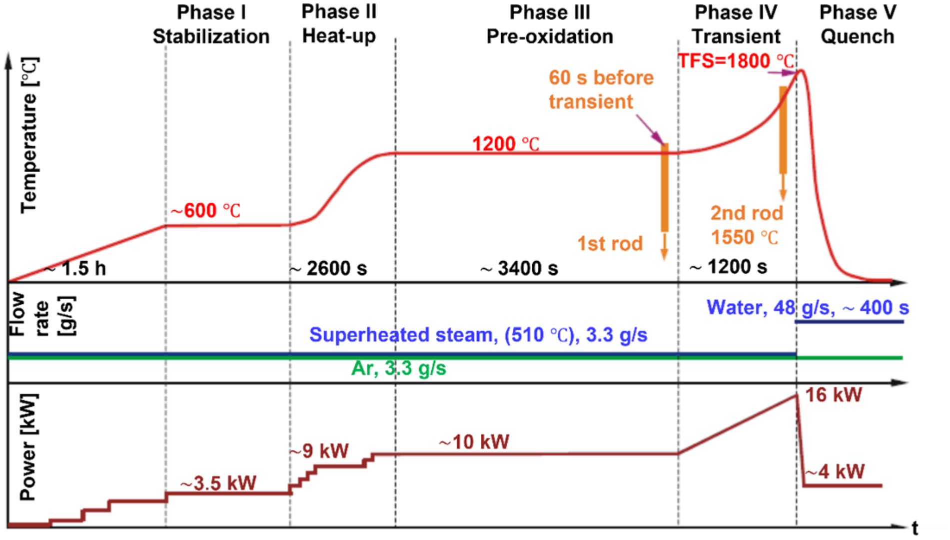
Motivation

- KIT strategy for severe accident (SA) analyses → continuous improvement of the codes to evaluate the progression and the radiological consequences of SAs in current and innovative NPPs
- Validation of codes is a key step in the KIT strategy
- The ASTEC integral code, developed by IRSN, is extensively employed at KIT
- **ASTEC validation against QUENCH experiments is continuously going on since long at KIT → almost all the QUENCH bundle tests analyzed**
- Current priorities in the research activities:
  - Further widening the range of application of ASTEC, i.e., VVER (Q-12) and BWR (Q-20)
  - Enable the safety assessment of the innovative reactor concepts, i.e., SMRs, expected to employ ATF cladding materials

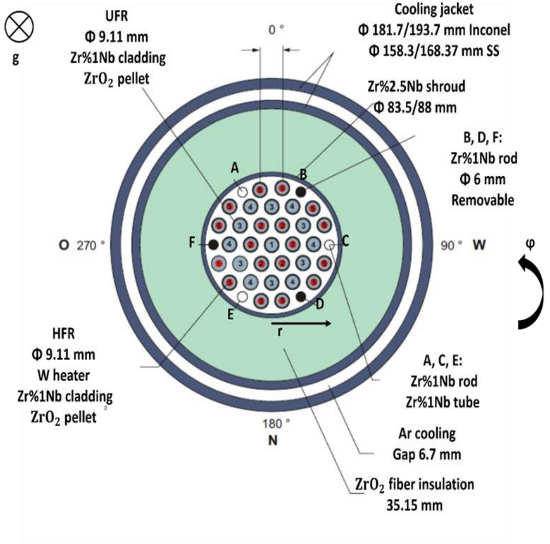
ASTEC Validation against QUENCH-12

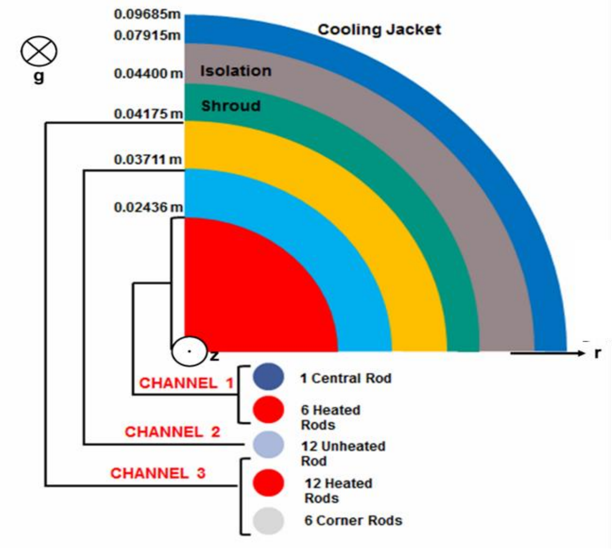
- Framework: assessment of an ASTEC dataset of a generic VVER-1000 NPP
- QUENCH-12: VVER-type fuel assembly arrangement
  - Reflooding of pre-oxidized heated rods bundle

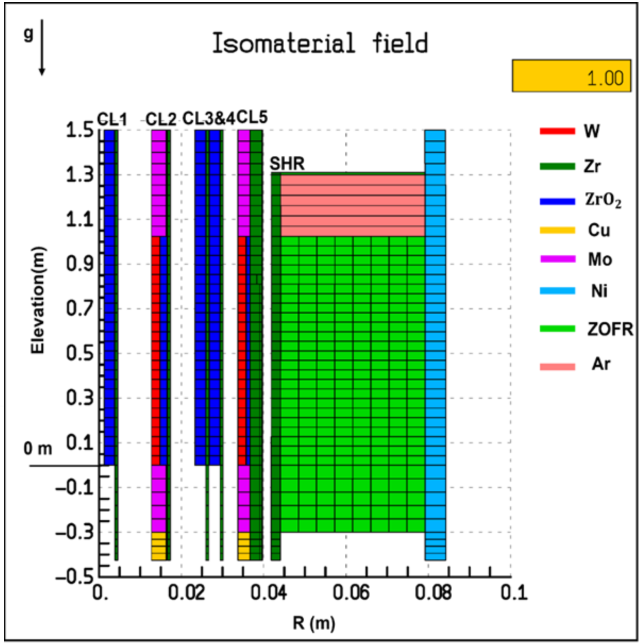




ASTEC model of the QUENCH-12 Test







- **All the ASTEC models activated**
- Zr material data employed instead of Zr-1%Nb → work in progress at KIT

A. K. Mercan, F. Gabrielli and V. H. Sanchez-Espinoza, "Validation of ASTEC2.1 using QUENCH-12 for VVER-Reactors," NED 395, 111840, 2022

ASTEC Results vs. QUENCH-12 Experiment

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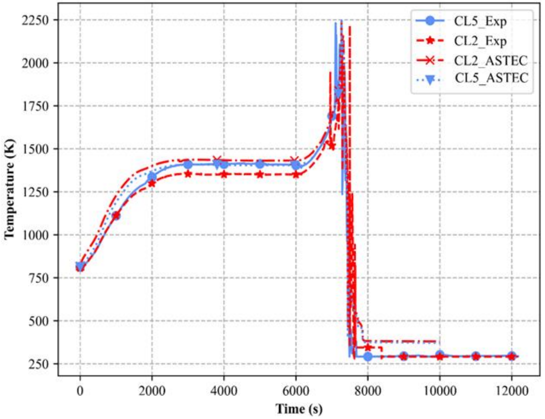
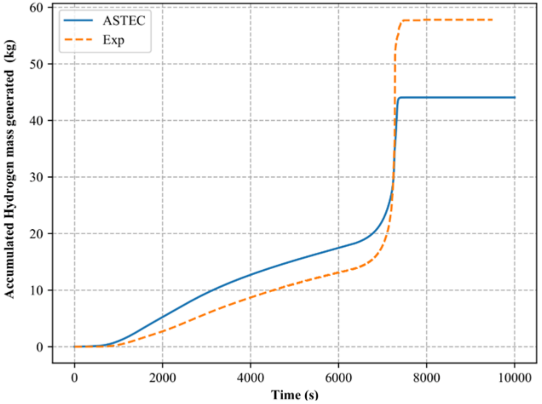
Heated rods @950 mm height



Hydrogen production

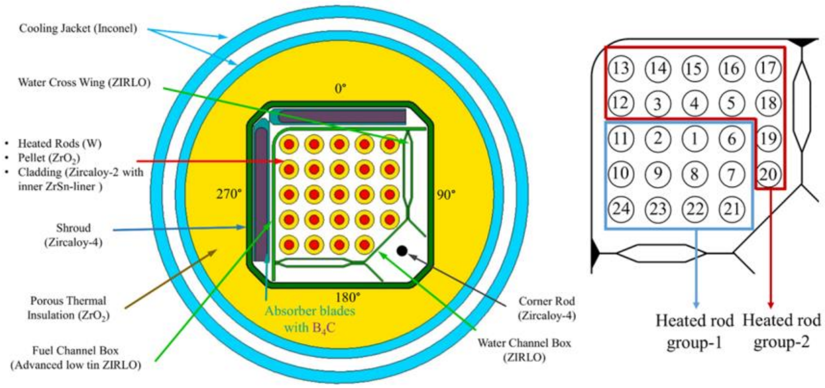


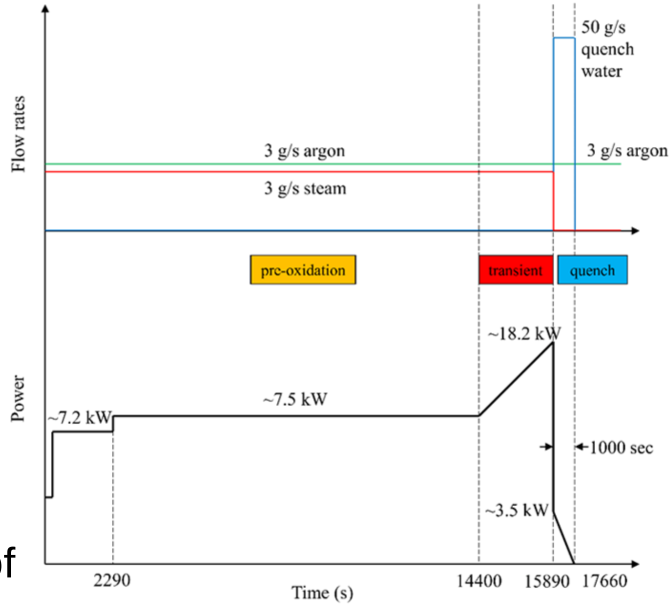
- **Good agreement on the temperatures of heated and un-heated rods**
- **Hydrogen production**
  - **Good agreement up to the beginning of the quenching phase**: 34.2 g (ASTEC) vs. 34.7g (Exp.)
  - **Underestimation during the quenching phase**: 9.9 g (ASTEC) vs. 23.1 g (Exp.) → due to the use of Zr-4 instead of Zr-1%Nb
- **The code is able to catch the physical phenomena of the experiment**

A. K. Mercan, F. Gabrielli and V. H. Sanchez-Espinoza, "Validation of ASTEC2.1 using QUENCH-12 for VVER-Reactors," NED 395, 111840, 2022

ASTEC Validation against QUENCH-20

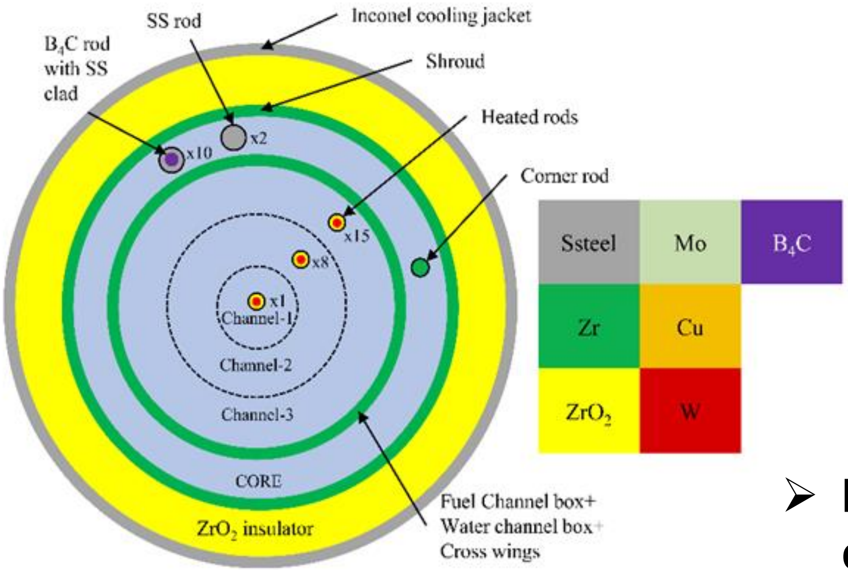
- **Framework: assessment of an ASTEC dataset of a generic model of the Peach Bottom BWR NPP (first-of-its-kind)**
- **QUENCH-20: Test Bundle Cross Section (1/4 SVEA 96 OPTIMA-2)**



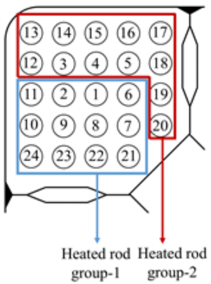


1. Pre-oxidation phase: power at 7.5 KW, steam and Ar flows
2. Transient phase: Electric power increases up to 18.2 kW
3. Quench phase: 50 g/s quench water Injected at the end of the transient phase, steam flow off

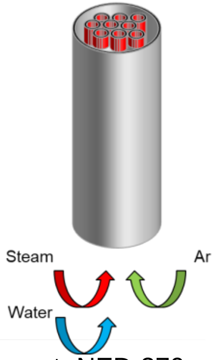
ASTEC model of the QUENCH-20 Test



- **Efforts to properly model the power distribution in the bundle**



- **The electrical power is not the same for each rod**
- **Boundary conditions from the experiment**
- **All ASTEC models activated**



O. Murat, V.H. Sanchez-Espinoza, S. Wang, J. Stuckert, Preliminary validation of ASTEC V2.2.b with the QUENCH-20 BWR bundle experiment, NED 370, 2020

ASTEC Results vs. QUENCH-20 Experiment

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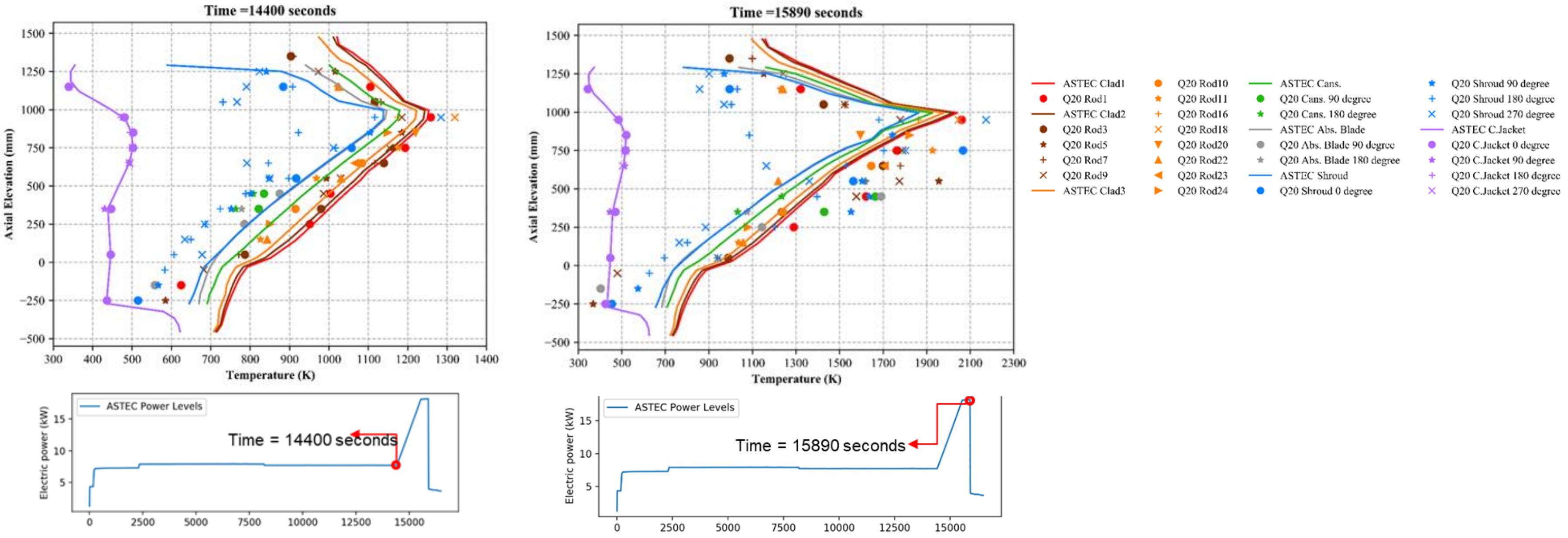
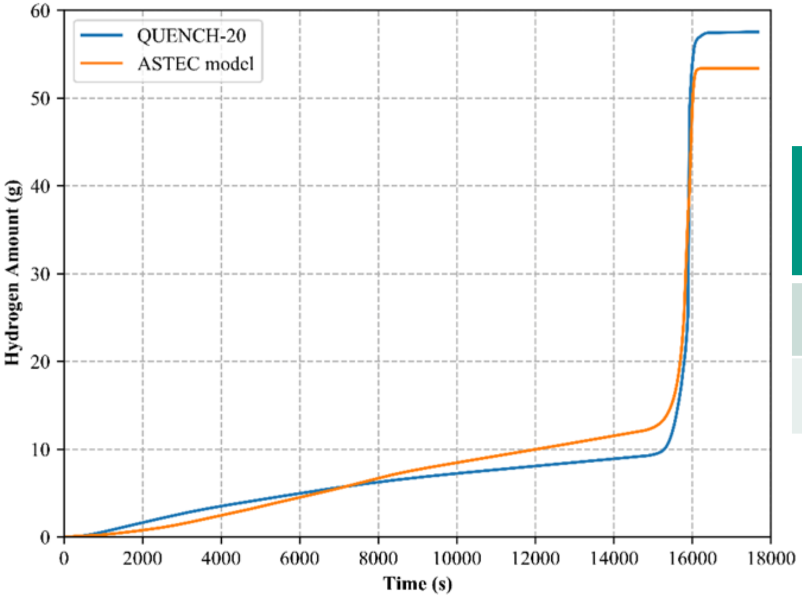


- Considering the challenges in modelling the geometrical peculiarities of bundle, **ASTEC reasonably well reproduces the temperature of the structures during the transient**

O. Murat, V.H. Sanchez-Espinoza, S. Wang, J. Stuckert, Preliminary validation of ASTEC V2.2.b with the QUENCH-20 BWR bundle experiment, NED 370, 2020

ASTEC Results vs. QUENCH-20 Experiment



Contribution to H_2 production	Exp. [g]	ASTEC [g]
Total	**57.4**	**53.4**
B4C oxidation	**10.0**	**9.48**

➢ **ASTEC results on both the total and B4C contribution to the hydrogen production during the test are in good agreement with the experiment**

O. Murat, V.H. Sanchez-Espinoza, S. Wang, J. Stuckert, Preliminary validation of ASTEC V2.2.b with the QUENCH-20 BWR bundle experiment, NED 370, 2020

Uncertainty and Sensitivity Analyses (U&Sa)

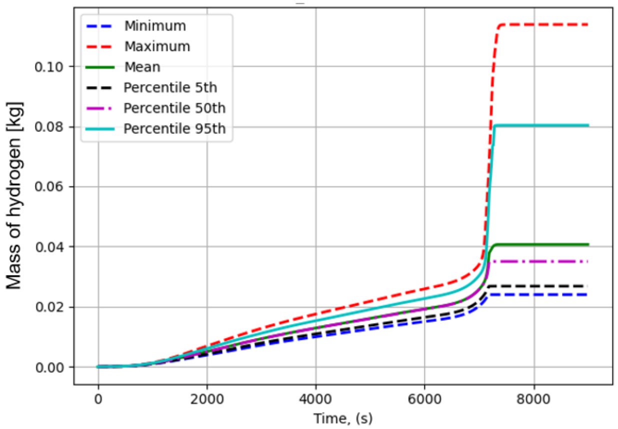
- **U&Sa of the ASTEC results became part of the calculation route in the KIT strategy for SA analyses**
- **The application of U&Sa methods to the ASTEC results for the QUENCH tests play a key role in order to:**
  - **Testing the U&S methodologies**
  - **Identifying bottlenecks in the code, when developing/employing new models devoted to new materials, i.e. ATF**
- **The KArlsruhe Tool for Uncertainty and Sensitivity Analyses (KATUSA) has been developed at KIT**
- **The ASTEC/KATUSA has been used for the QUENCH-08 and QUENCH-06 analyses**

Uncertainty and Sensitivity Analyses (U&Sa)

- The **U&Sa of the results of integral codes for the QUENCH-06** has been **selected as test case (Task 1)** in the IAEA CRP I31033 'Advancing the State-Of-Practice in Uncertainty and Sensitivity Methodologies for Severe Accident Analysis in Water Cooled Reactors' (2019-2024)
- Participants to the Task: KIT (coordination), ENEA, IBRAE, LEI

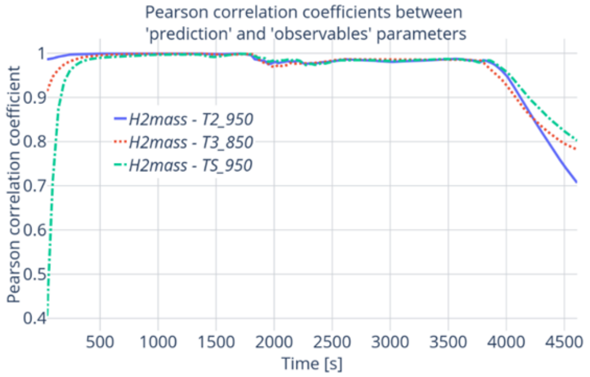
- 5 Figure-of-Merits selected (H_2 production, temperatures, oxide scales)
- 23 uncertainty parameters selected and the corresponding PDFs characterized
- The TECDOC is in the publication process

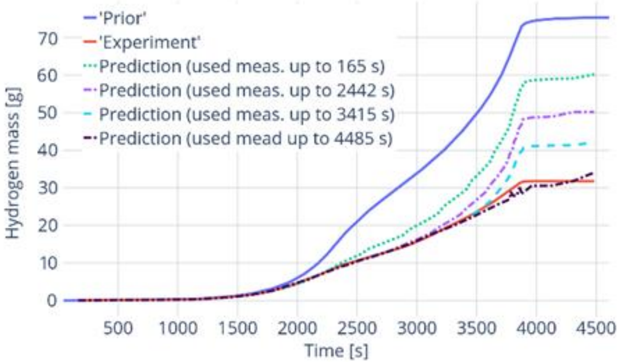
Simple statistics (ASTEC)



U&Sa and Prediction of H2 Production (QUENCH-08)

- Framework: Development of a tool for fast source term (ST) predictions based on a database of results from the ASTEC code (German WAME project, **accomplished**)
- Fast Source Term Code (FSTC) developed at KIT
  - U&Sa+Data Assimilation algorithm based on MOCABA (developed by Framatome GmbH)
  - Goal: iteratively use the measurements and previous predictions to construct the new one
- Before moving to NPPs applications, FSTC tested on the QUENCH-08 experiment
- An ASTEC database of 600 simulations assessed
- The ASTEC/FSTC allows predicting the hydrogen mass by using the TC measurements





A. Stakhanova, F. Gabrielli, V.H. Sanchez-Espinoza, A. Hoefer, E.M. Pauli, Application of the MOCABA algorithm and the FSTC tool for source term predictions during severe accident scenarios, Annals of Nuclear Energy, 184, 2023.

ASTEC Modelling of QUENCH ATF-Related tests

- **Large efforts on the analysis of the QUENCH ATF-related bundle tests on-going**
- **Framework: OECD/NEA QUENCH-ATF and IAEA CRP ATF-TS**
- Current approach in the ASTEC modelling: modifying the material database by including the correlations for such materials, i.e. FeCrAl

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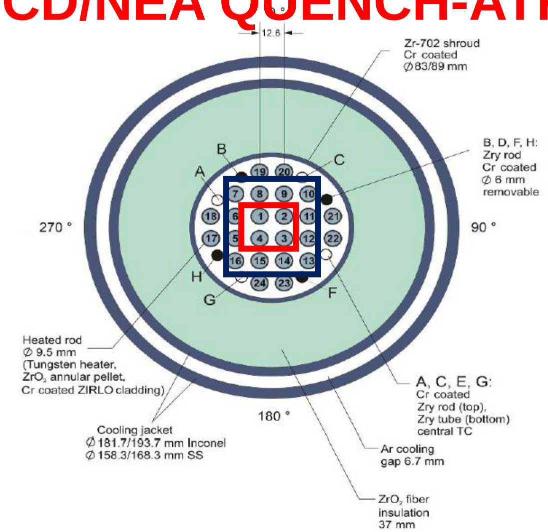
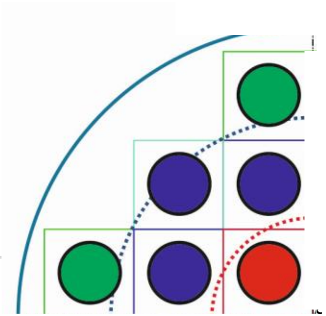
STRUCTURE MODEL NAME 'BEST-FIT' LAW 'COEFF' VARIABLE 'T' VUNIT 'K' RUNLOW 0. RUNUPP 5000.
  SRG VALUE AGAIN 9.62D-10 BGAIN 0.0 ATHIC 2.252D-13 BTHIC 0.0 MODEL 0.5 TERM
  X  1473.K
  SRG VALUE AGAIN 3.0D+11 BGAIN 5.94354D5 ATHIC 3.371D3 BTHIC 5.94354D5 MODEL 0.5 TERM
  X  1648.K
  SRG VALUE AGAIN 2.4D+08 BGAIN 3.52513D5 ATHIC 0.008682D0 BTHIC 3.52513D5 MODEL 0.5 TERM
 END
```

- **Mid-term approach: development and implementation in ASTEC of an oxidation model for new materials (currently efforts devoted to FeCrAl)**

ASTEC Model of the QUENCH-ATF1 Test

- **OECD/NEA QUENCH-ATF Project**

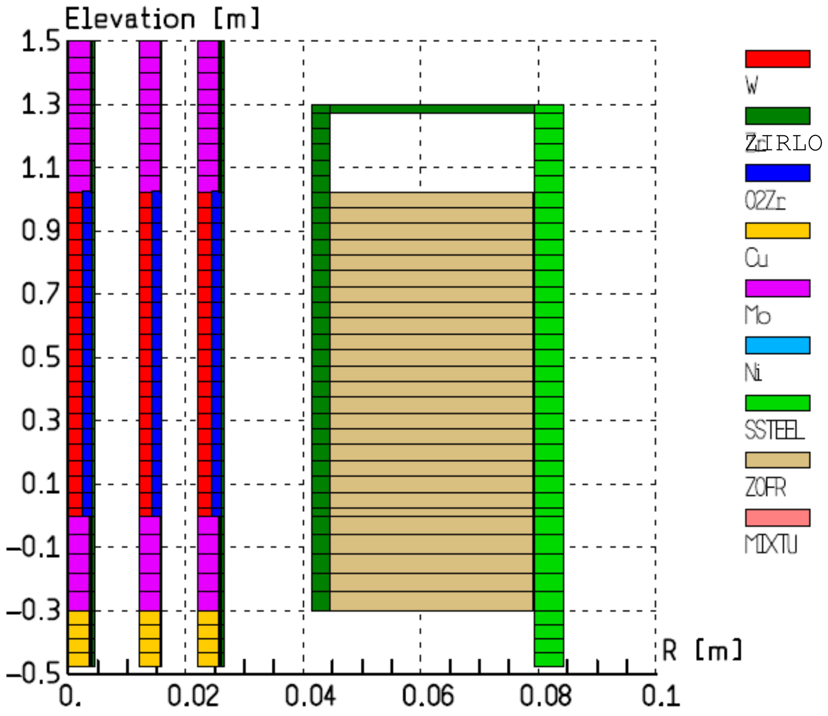




Ch. 3, 8 rods, r_{ext}= 41.5 cm

Ch. 2, 12 rods, r_{ext}= 28.4 cm

Ch. 1, 4 rods, r_{ext}=14.2 cm



Oxidation Model

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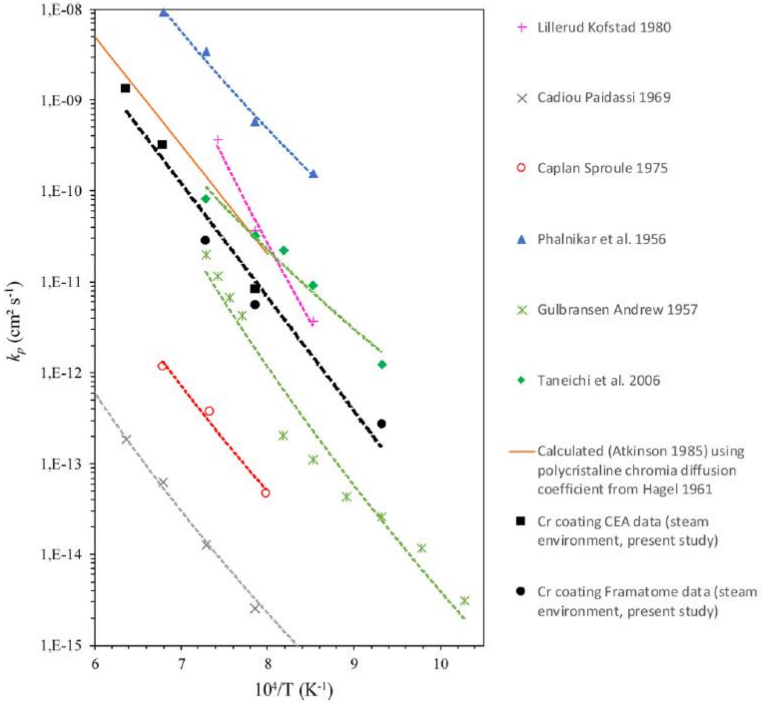


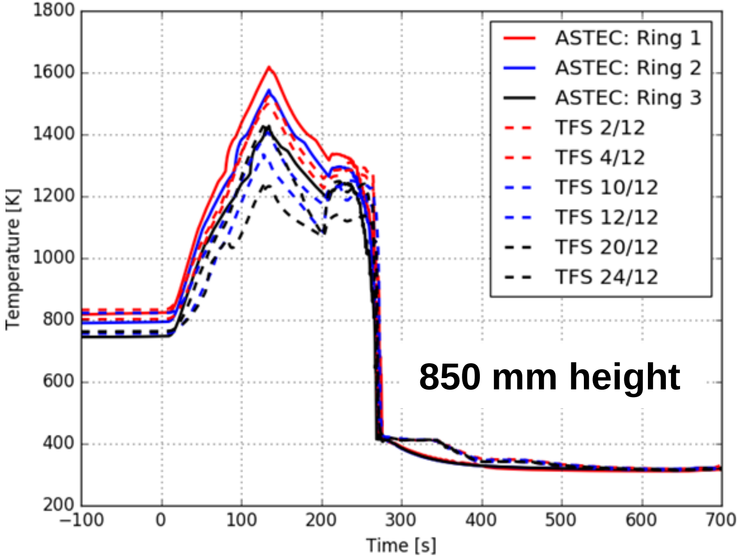
- **Brachet data**
- **Fitting functions for weight gain and thickness grown of the oxide layer provided by J. Stuckert**

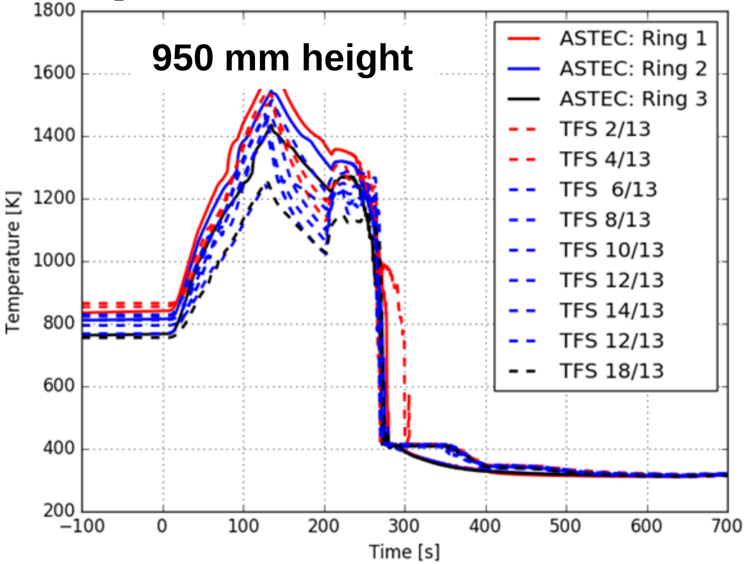
$$\delta = 0.00377 \cdot e^{-\frac{123783}{R \cdot T}} \cdot \sqrt{t}$$

$$\Delta m = 6.19 \cdot e^{-\frac{123783}{R \cdot T}} \cdot \sqrt{t}$$

Brachet, J.-C., et al., 2020. High temperature steam oxidation of chromium-coated zirconium-based alloys: Kinetics and process, Corrosion Science 167 (2020) 108537..

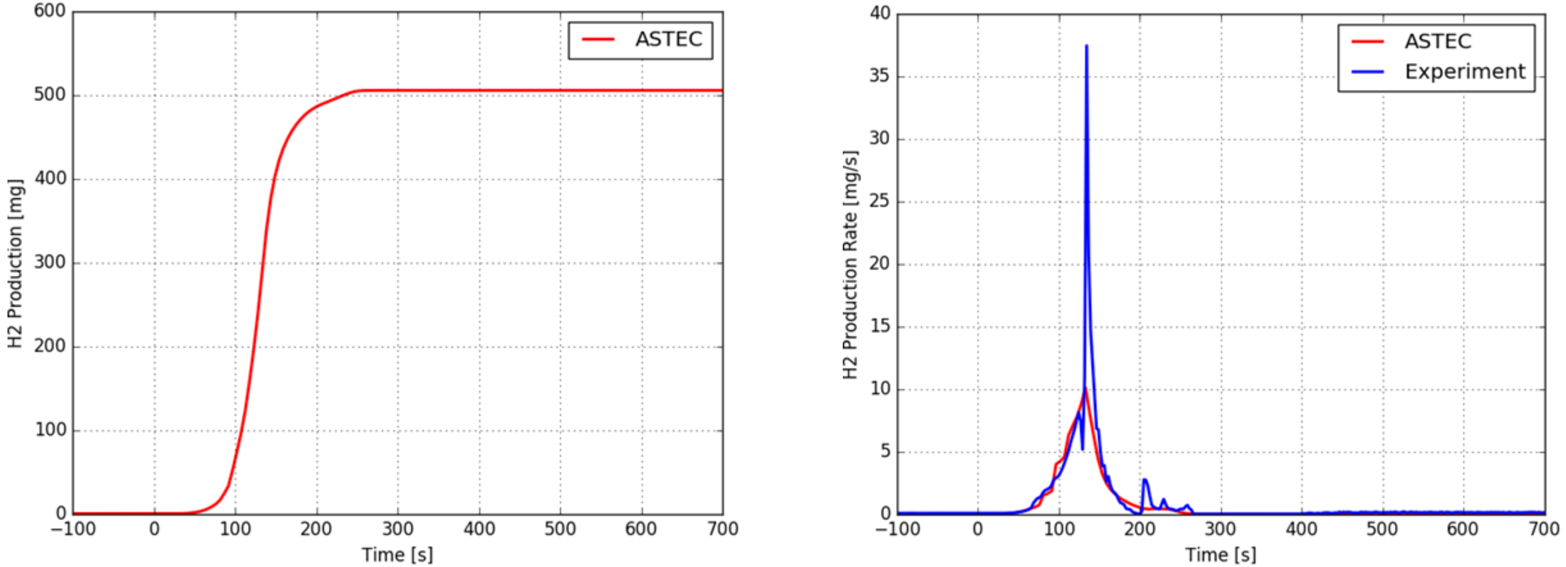
ASTEC Model: Results – Clad Temperature





- Ring#1: reasonable agreement
- Ring#2: deviations @850 mm height (~200 degree), reasonable for some TCs @950 mm
- Ring#3: large deviations (up to~200 degree)
- Good agreement on the radial shape

ASTEC Model: Results – H2 production

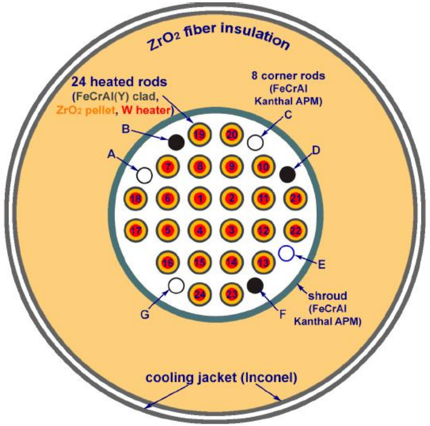


- **Large deviation on the maximum H2 production rate**
- **Very good agreement on the starting time of H2 production and on the kinetics behavior**

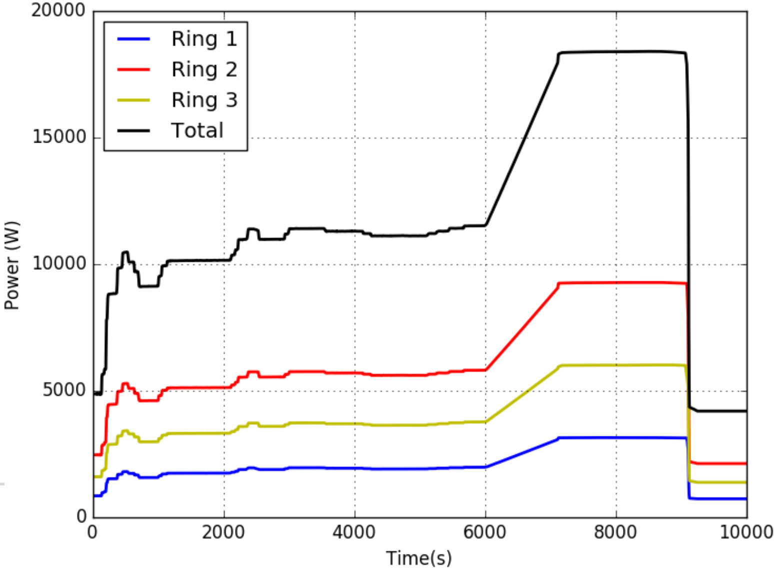
QUENCH-19 Test

➢ IAEA ATF-TS Project

- ➢Phase 1: heating up to ~600 °C (4 kW)
- ➢Phase 2: power increase up to 11.5 kW (pre-oxidation)
- ➢Phase 3: power increased up to 18.12 kW (5 W/s) (T_{pct}~1500 °C)
- ➢Phase 4: power reduced to 4.1 kW

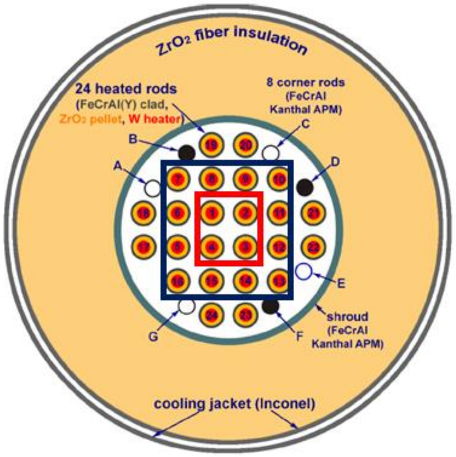


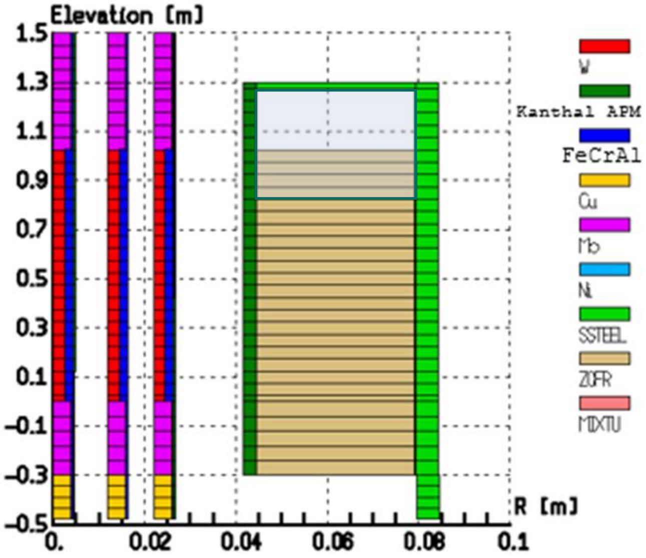
- ➢Atmosphere of Ar (3.45 g/s) and superheated steam (3.6 g/s).
- ➢Reflooding at ~9100 s
  - ➢Fast initial injection of 4 kg of water
  - ➢Slow injection 48 ~ g/s of water

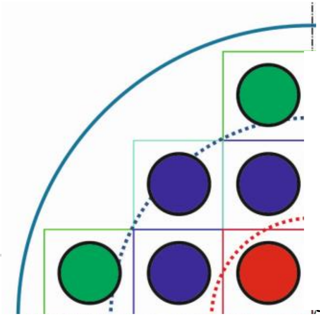


ASTEC Model of the QUENCH-19 Test

➢ IAEA ATF-TS Project







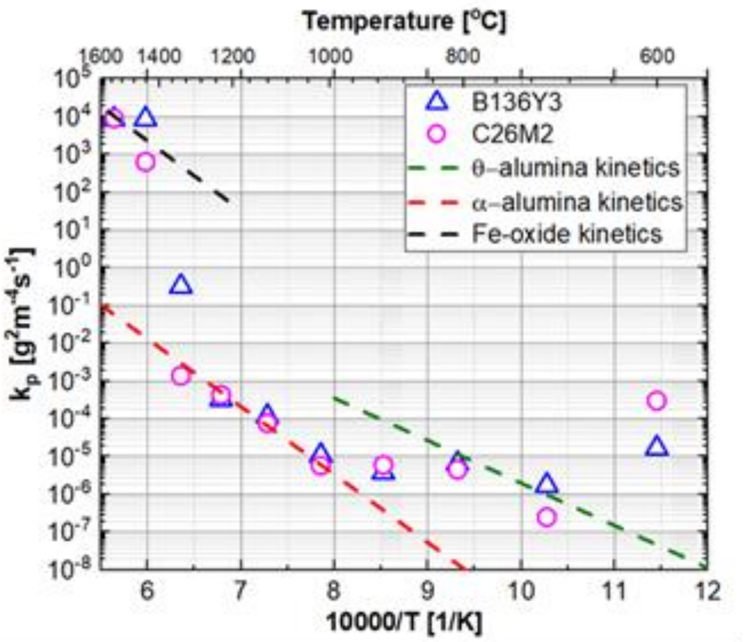
Ch. 3, 8 rods, r_{ext}= 41.5 cm

Ch. 2, 12 rods, r_{ext}= 28.4 cm

Ch. 1, 4 rods, r_{ext}=14.2 cm

➢ Accidental presence of 4 l water the gap between the shroud and the cooling jacket modelled

ASTEC: FeCrAl Oxidation Model



- **Fitting functions for weight gain provided by J. Stuckert**

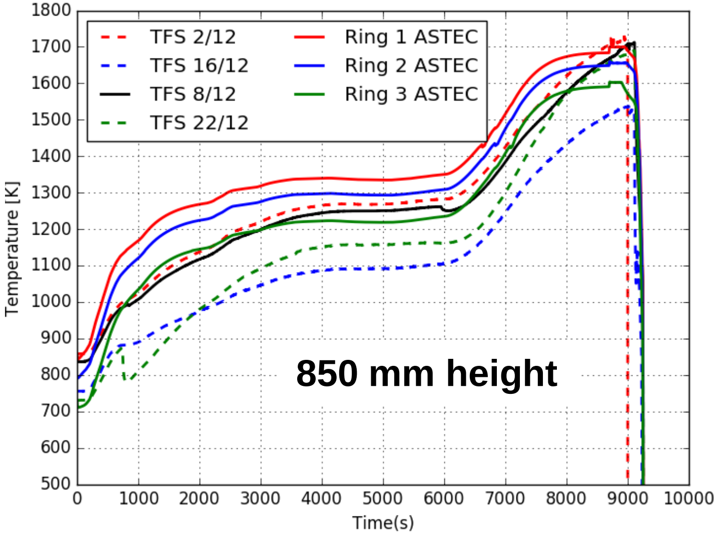
$$K = \begin{cases} 9.62 \times 10^{-12}\,[\mathrm{g^2/cm^4 s}], & T \leq 1473\ \mathrm{K} \\ A_B \exp\left(\frac{-E_B}{RT}\right), & 1473 < T < 1648\ \mathrm{K} \\ A_{Fe} \exp\left(\frac{-E_{Fe}}{RT}\right), & T \geq 1648\ \mathrm{K}\ (melting\ point\ of\ FeO) \end{cases}$$

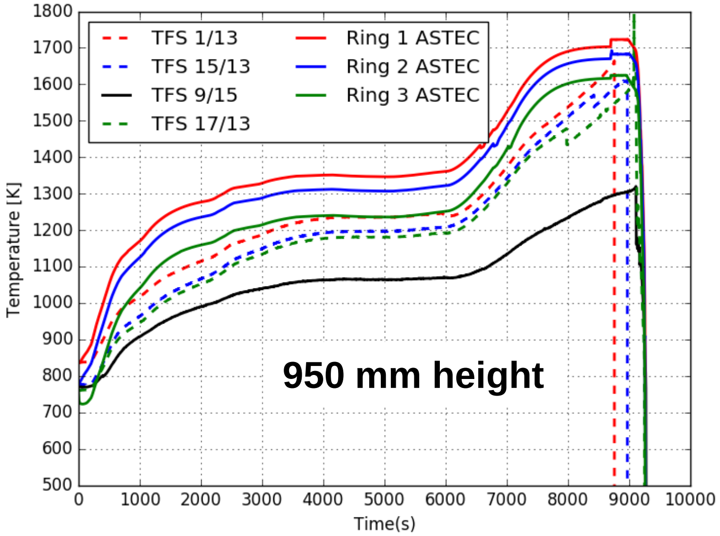
$A_B = 3 \cdot 10^9$ g²/cm⁴ s **$E_B = 594354$ J/mol**

$A_{Fe} = 2.4 \cdot 10^6$ g²/cm⁴ s **$E_{Fe} = 352513$ J/mol**

C. KIM, C. TANG, M. GROSSE, M. STEINBRUECK, C. JANG, Y. MAENG, „OXIDATION KINETICS OF NUCLEAR GRADE FeCrAl ALLOYS IN STEAM IN THE TEMPERATURE RANGE 600-1500°C", TopFuel 2021.

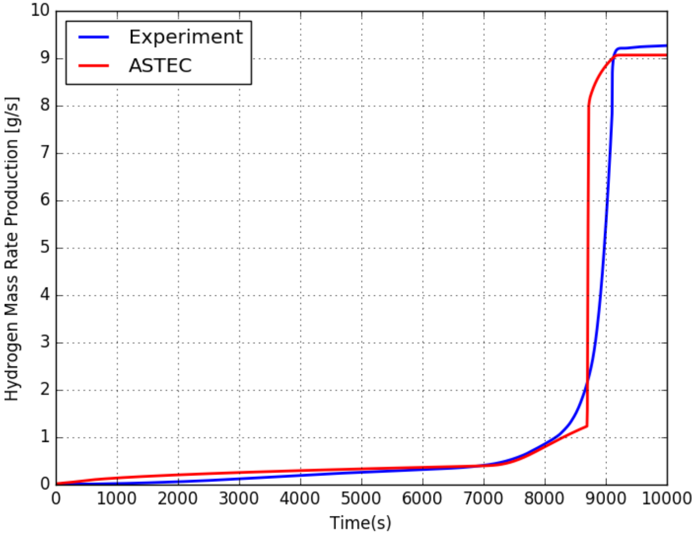
ASTEC Results: Clad Temp. @850 and @950 mm Height

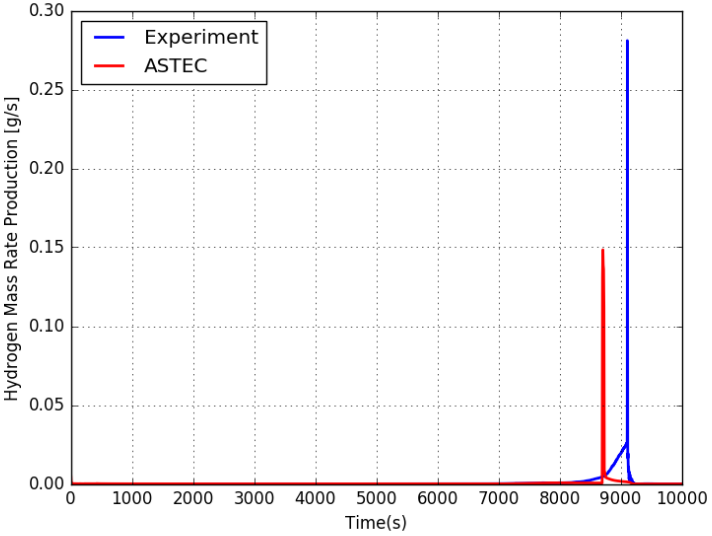




- Results exceed the exp. of about 100 degree in the pre-oxidation phase in Ring 1 (@850 mm) and in the Ring 1 and 2 (@950 mm height)
- Better agreement in Ring 2 and 3 (@850 mm) and Ring 3 (@950 mm)
- **Maximum temperatures reasonably well reproduced**

ASTEC Results: Hydrogen Production





- **The final amount of H2 is reasonably well reproduced**
- ASTEC results show a good agreement with exp. up about 8000 s
- Escalation is anticipated in time with about 50% of the mass rate compared with the experiment
- **'Smooth' kinetics behavior is not reproduced**

Conclusion

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- The validation activity of the ASTEC code against the QUENCH bundle tests is going on since long at KIT
- **The activity is a pillar of the KIT strategy on the analysis of hypothetical SAs in current and innovative NPPs**
- **ASTEC is able to properly reproduce the key phenomena and/or the experimental results of the QUENCH bundle tests**
- Efforts are currently devoted to analyze the QUENCH tests employing ATF materials in the frame of:
  - **The OECD/NEA QUENCH-ATF project**
  - **The IAEA T12032 CRP ‘ATF-TS’**
  - **The development and the implementation in ASTEC of a physical model for the oxidation of FeCrAl cladding materials (tight connection with IRSN and the QUENCH team)**

Acknowledgement

The authors wish to acknowledge the QUENCH team for the great support to the KIT/INR computation team

Special thank to J. Stuckert, M. Steinbrück, and M. Große for their continuous support, suggestions, and availability