

DEVELOPMENT OF MELCOR v2.2 INPUT FOR THE SIMULATION OF QUENCH-06 EXPERIMENT

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CONTENTS

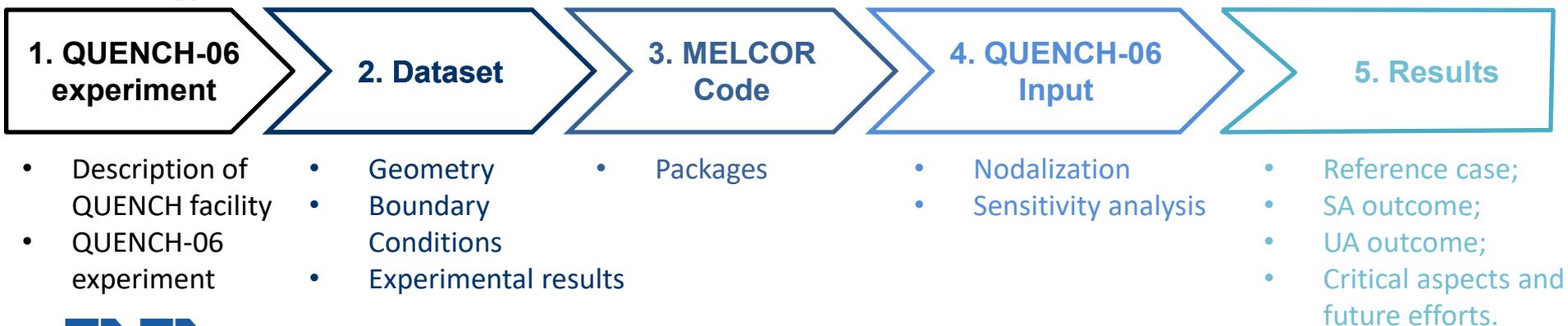
Framework:

IAEA CRP «*Advancing the State-of-Practice in Uncertainty and Sensitivity methodologies for Severe Accident Analysis in Water-cooled reactors*» is aimed to achieve significant improvement in sophistication and quality of SA analyses performed by the participants with well-developed knowledge, adequate simulation capabilities and long years of relevant practice. QUENCH-06 is one among the proposed exercises.

Goals of the work:

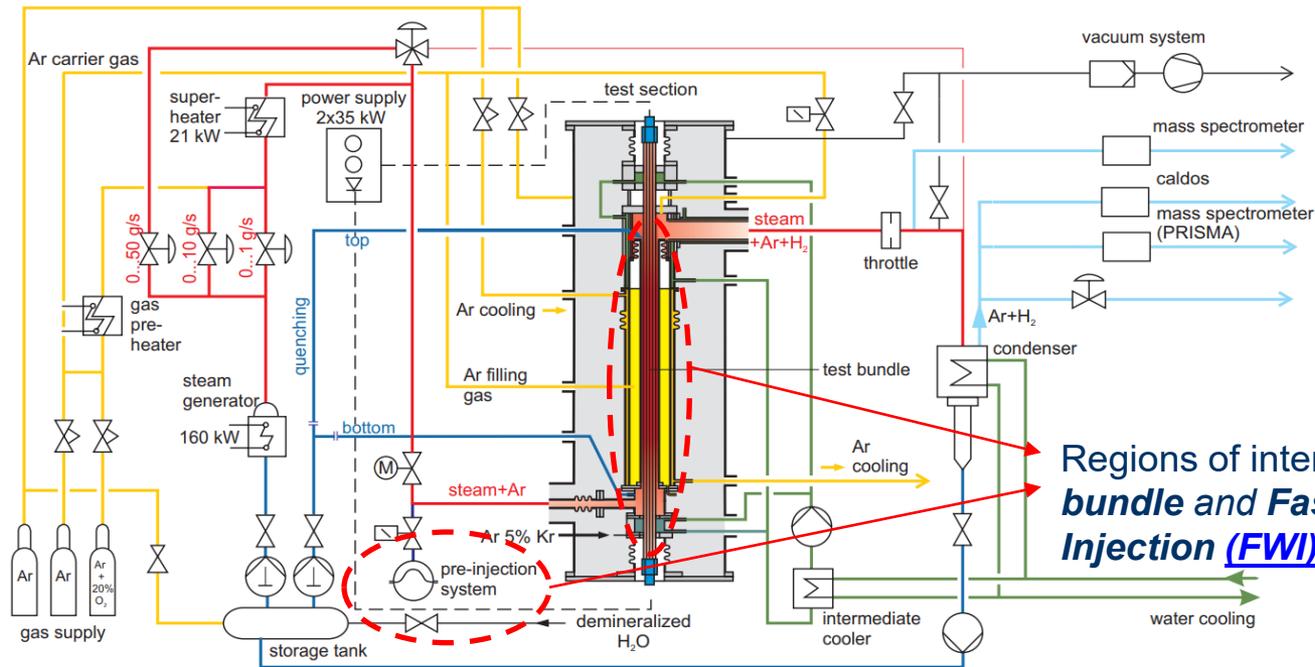
- Independent user validation of *Core Heat up, Zircaloy-Steam Oxidation* and *Degradation* models embedded into best estimate MELCOR code employing the experimental dataset provided by QUENCH-06 test;
- Sensitivity analysis (SA) adopting several Zircaloy-Steam oxidation reaction rates;
- Uncertainty analysis (UA).

Methodology:



QUENCH facility

QUENCH is a series of scaled down, separate effect tests conducted at KIT

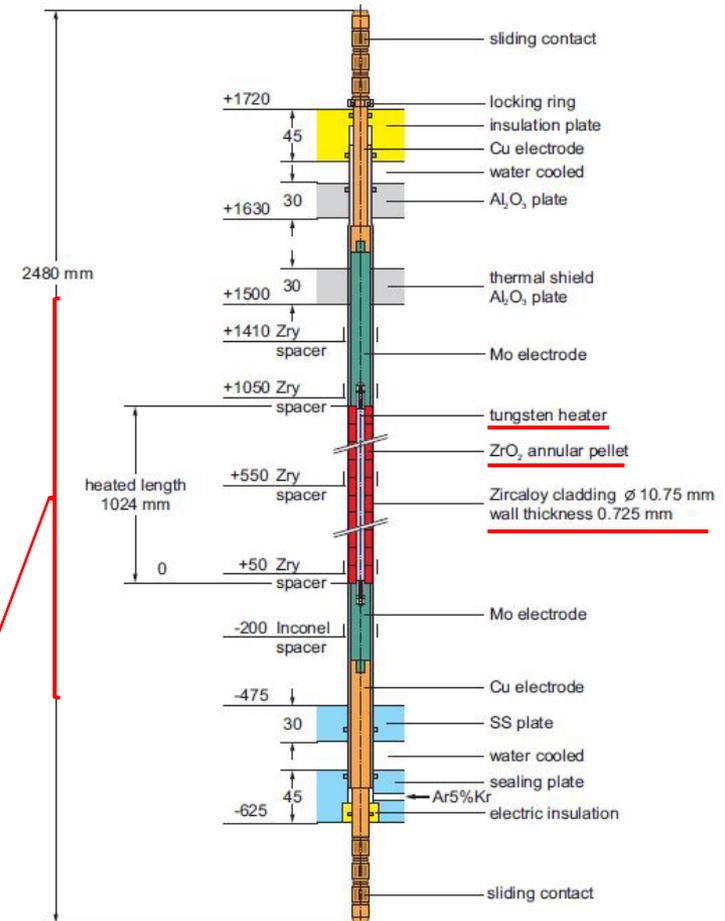
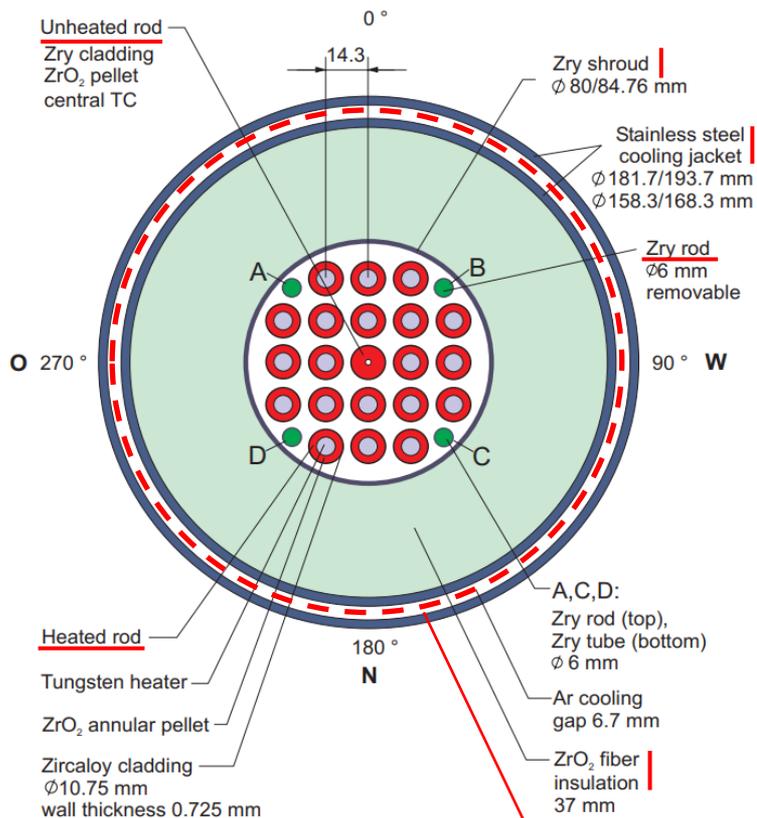


Regions of interest: **Test bundle** and **Fast Water Injection (FWI) system**.

Goals of **QUENCH-06**:

- Evaluate the hydrogen build-up in a simulated Desing Basis Accident from Zircaloy oxidation during:
 1. a cool-down phase carried out by just steam and argon flows;
 2. quenching with subcooled water.
- Determine the behaviour of pre-oxidized LWR-like fuel rod on cooling down with water.

TEST BUNDLE AND FUEL ROD SIMULATORS



MELCOR QUENCH-06 Input Domain

ϕ : [0 m, 0.1683 m]

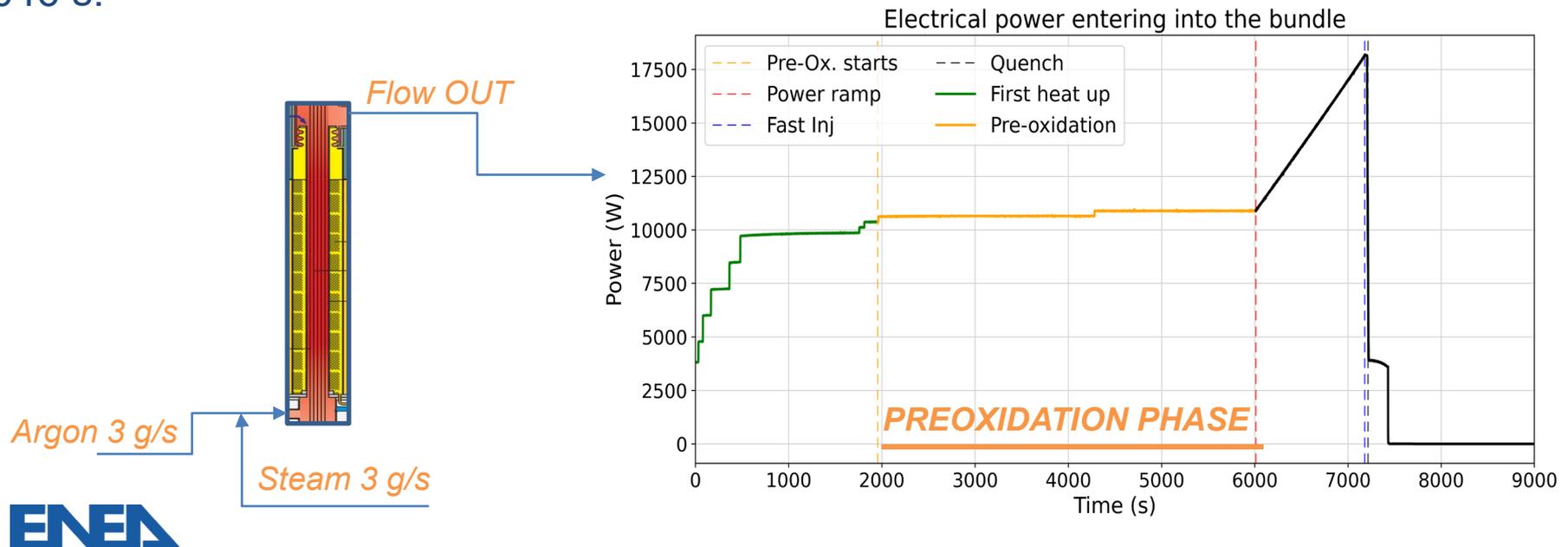
ΔH : [-0.47658 m, 1.5 m]

TEST PHASES: PREPARATION AND PREOXIDATION

Bundle is heated by a stepwise increase of electrical power from room temperature up to about ~ 873 K, while crossed by flowing argon (3 g/s) and steam (3 g/s) coming from the bottom. System status is kept for 7200 s.

After this stabilization period, ($t = 0$ s) measurements are turned on and power is ramped up from 4 kW to 11 kW without any changes in mass flow rates.

Once the bundle has reached ~ 1473 K (target value), **Preoxidation** of the Zry claddings and shroud occurs, while temperature is maintained by control systems for 4046 s.

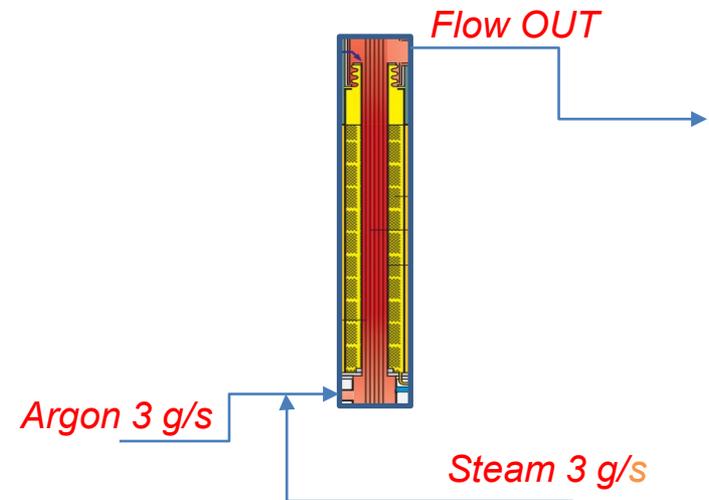
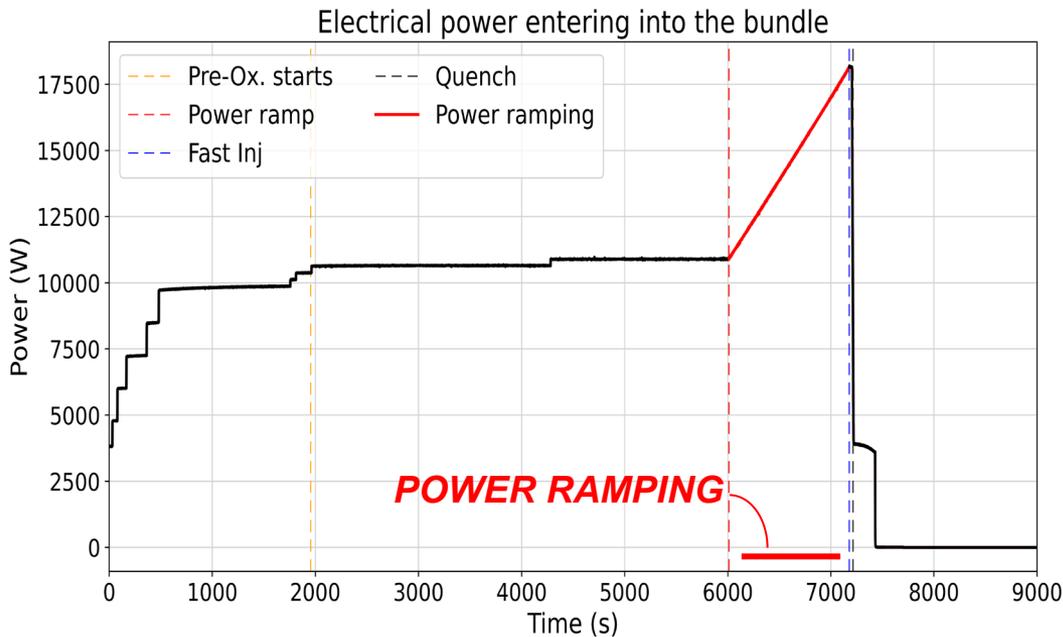


TEST PHASES: POWER RAMPING

At the end of pre-oxidation period, a **Power ramping** begins, where power is steeply increased until the **quenching condition** is satisfied (**t = 7179 s**):

- a minimum of three rod thermocouples should have exceeded ~1973 K, and the central rod thermocouple should have reached ~1873 K at this time.

This phase is characterized by the highest hydrogen production rate of all the experiment.



TEST PHASES: QUENCHING

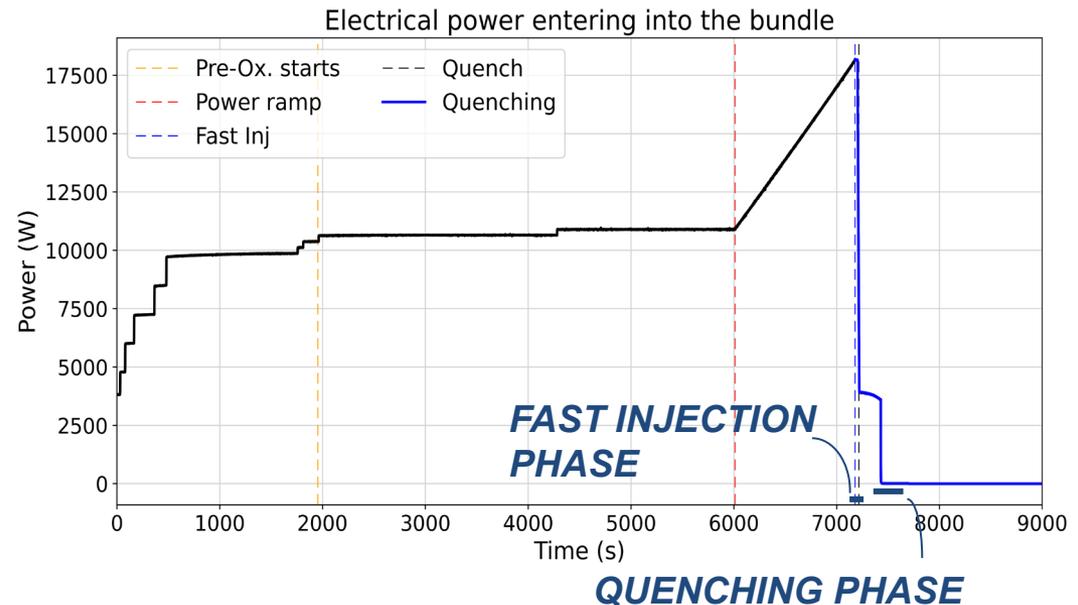
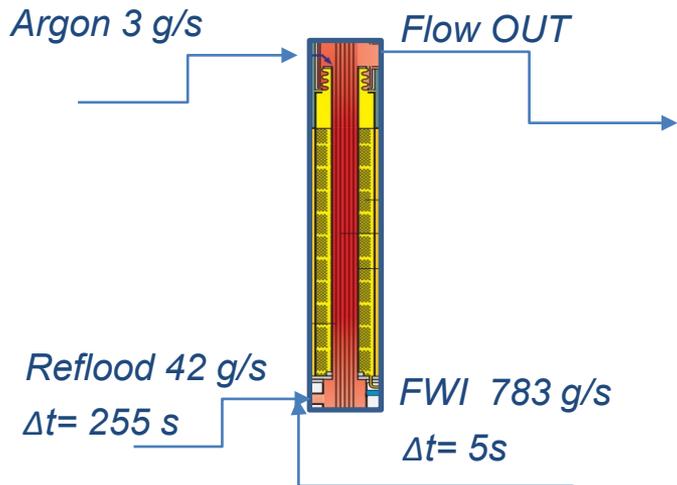
Quenching phase begins by turning off bottom injections and switching the argon flow rate to the head of the bundle.

Fast injection (FWI) system is activated at **$t = 7179.5$ s** for 5 s allowing 4 l of quench water (6 bar, 397 K) for pre-filling the pipes and the lower plenum.

With 30 s of delay (**$t = 7215$ s**), quenching water is pumped at a flowrate of 42 g/s for 255 s.

At **$t = 7205$ s** power is reduced to 4 kW to simulate decay power.

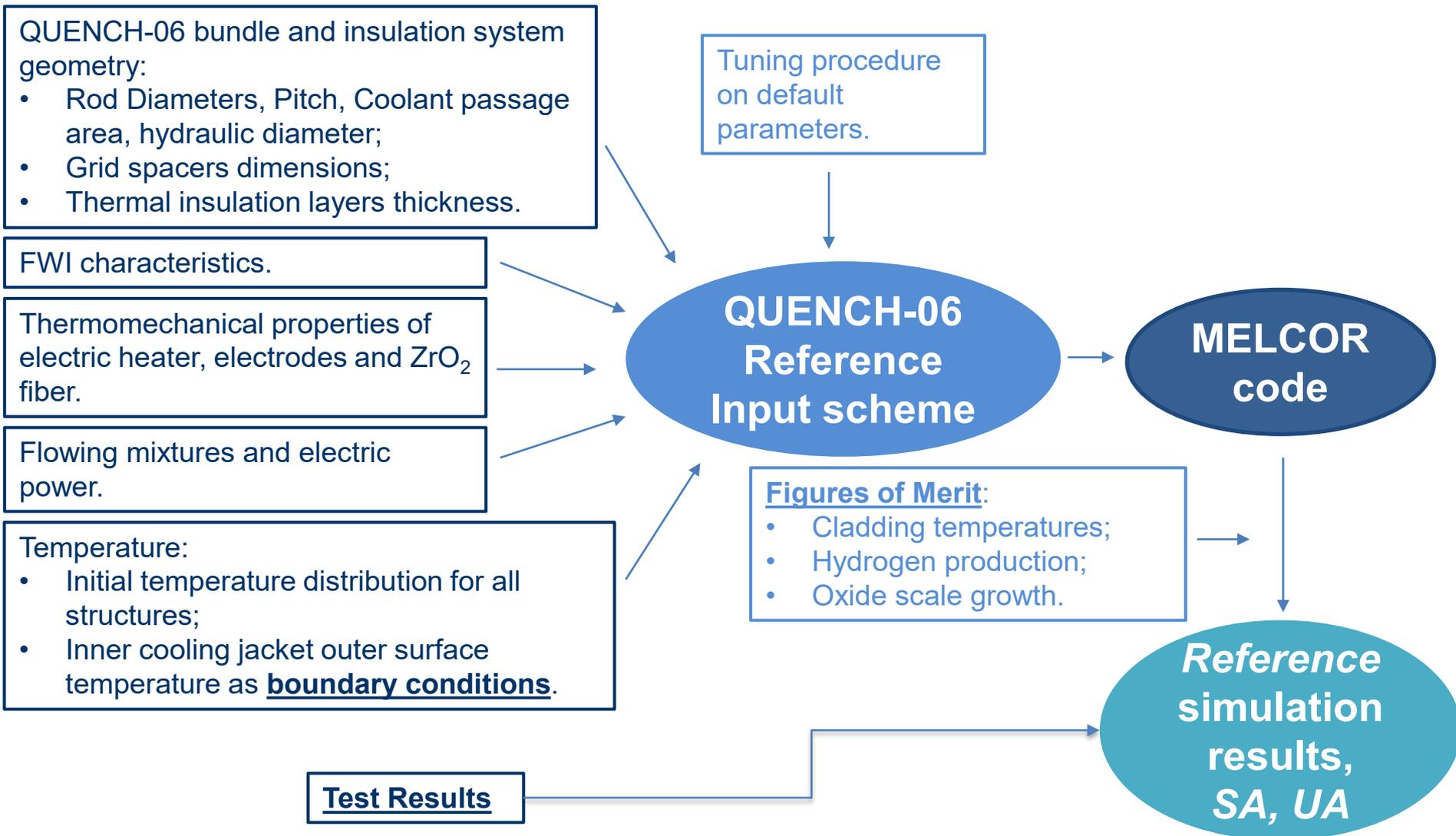
Around **$t = 7470$ s**, quenching is concluded, and power is set to zero.



QUENCH-06 EVENTS

Time [s]	Event	Flowing mixture
0	Test starts, heat up from 873 K to 1473 K	<ul style="list-style-type: none"> • 3 g/s steam [2 bar, 640 K] • 3 g/s argon [2 bar, 640 K]
1965	Preoxidation stage onset, power at 11 kW	“
6011	Power ramping	“
6620	Corner rod B withdrawal for metallographic analysis	“
7179.5	Reflood on-set	<ul style="list-style-type: none"> • 783 g/s FWI [6 bar, 370 K] • 3 g/s argon in bundle head [2 bar, 298 K]
7184.5	FWI ends	<ul style="list-style-type: none"> • 3 g/s argon in bundle head [2 bar, 298 K]
7215	Main quench, power to 4 kW	<ul style="list-style-type: none"> • 42 g/s water [2 bar, 397 K] • 3 g/s argon in bundle head [2 bar, 298 K]
7431	Power shutoff, quench ended	<ul style="list-style-type: none"> • 3 g/s argon in bundle head [2 bar, 298 K]
11420	Test termination	-

DATASET AND INPUT DEVELOPMENT



QUENCH-06 INPUT NODALIZATION

QUENCH-06 CVH-FL NODALIZATION (1)

TEST Control Volumes (CV)

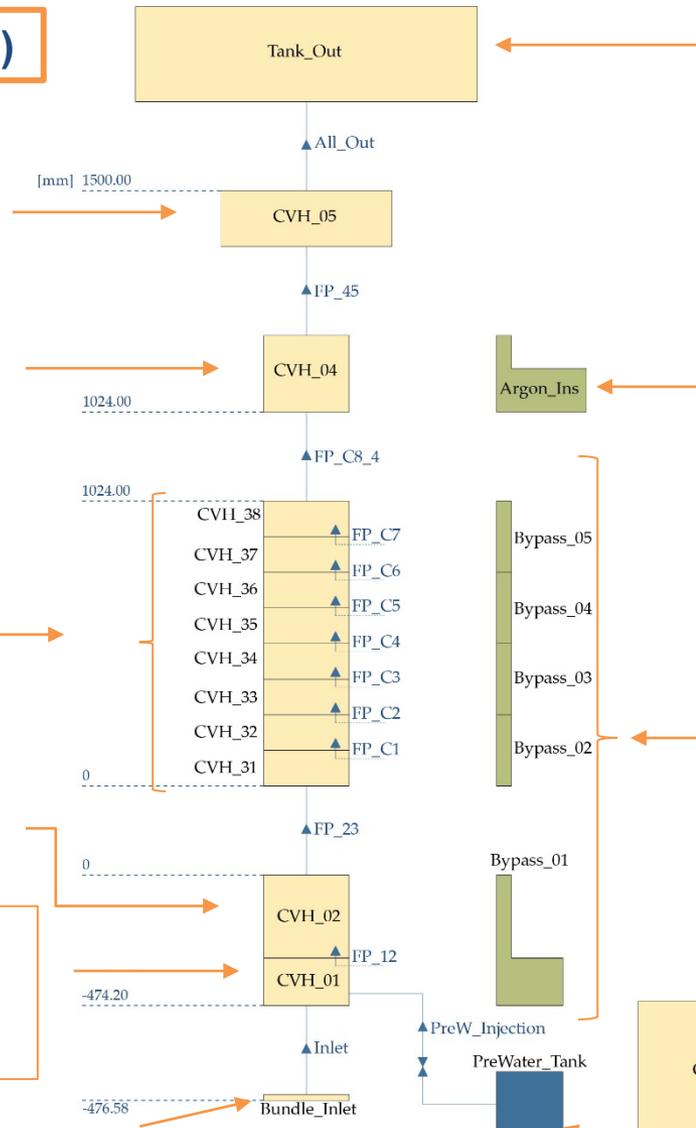
CVH_05: CV in correspondence of upper Mo electrode.
 • Post FWI Argon mass flow rate source

CVH_04: CV in correspondence of upper Mo electrode

CVH_31-38: CVs in active region

CVH_02: CV in correspondence of lower Mo electrode

CVH_01: CV in correspondence of Cu electrode
 • Steam, Argon and quenching water flow rates sources



TANK_OUT: it acts as a sink for all fluids crossing the test section (*TIME - INDEP* at 2 bar, 600 K)

ARGON_INS: argon insulation between the shroud and the cooling jacket. It acts also as bypass between 1.204m and 1.3m.

BYPASS: 5 thin dummy annuli between the Zry shroud and the ZO fiber (thickness 0.5 mm).

CONTAINMENT: Argon filled *TIME-INDEP* volume at 415 K.

BUNDLE INLET: for COR lower head

PREW_TANK: FWI system



QUENCH-06 CVH-FL NODALIZATION (2)

- Every **Test Section CV** is initialized as Both Pool and Atm, Active and with Non-equilibrium:
 - 1- Pool saturated (2 bar);
 - 2- Atm superheated (2 bar, 607 K).
- CVH_01: mass and temperature sources (steam, argon and quenching water) as TFs;
- CVH_05: mass and temperature sources of post quenching argon in-head injection as TFs;

As concerns flow paths linking **TEST CVs**:

$$\begin{aligned} \text{cross sectional area} &= 3.007 * 10^{-3} \text{ m}^2 \\ \text{hydraulic diameter} &= 0.01161 \text{ m} \end{aligned}$$

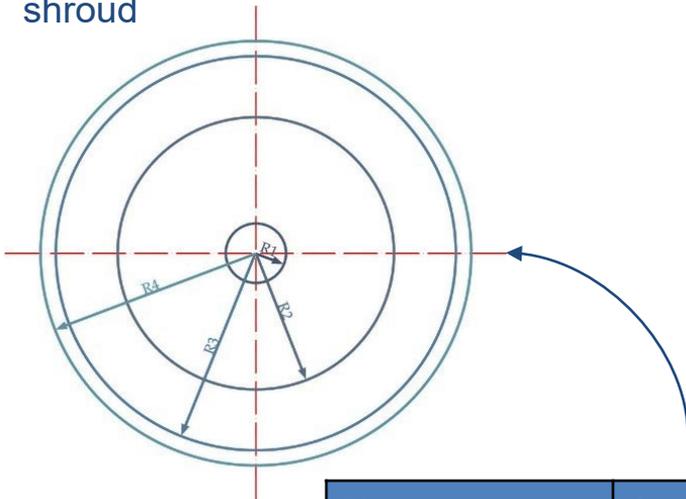
- Fast preinjection is triggered by the opening of a valve:
 1. Length, diameter and friction coefficient of the FL are determined after a sensitivity analysis in order to inject into the system 4 l of subcooled water in 5 s;
 2. **PreW_tank** CV is *TIME-INDEP* at 6 bar, *Only Pool*.
- **BUNDLE_INLET** is merely a dummy control volume that acts as lower plenum to match the COR nodalization of the lower head (it is *Active, Non Equilibrium* with *Both Pool and Atmosphere*).

QUENCH-06 COR NODALIZATION (1)

Test Bundle up to zircaloy shroud is nodalized in 4 concentric rings and 42 axial levels.

RADIAL NODALIZATION

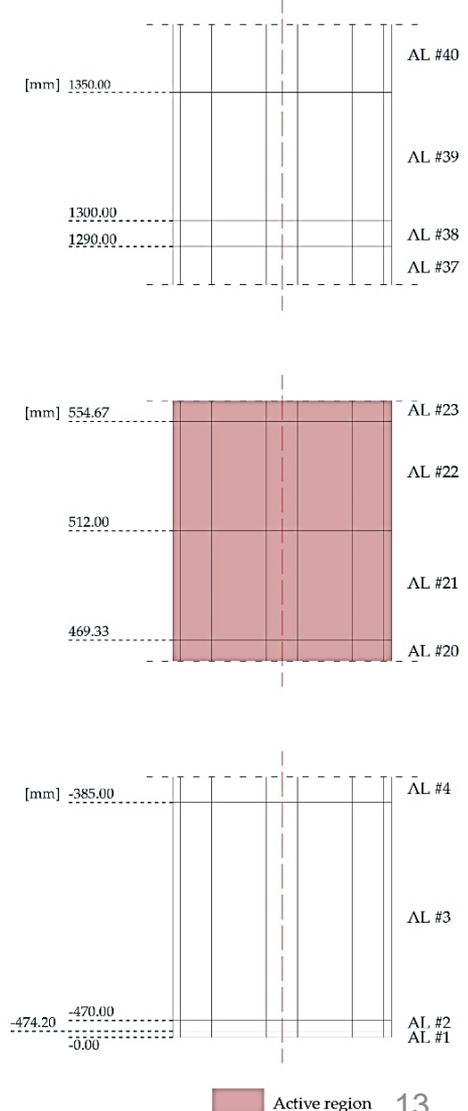
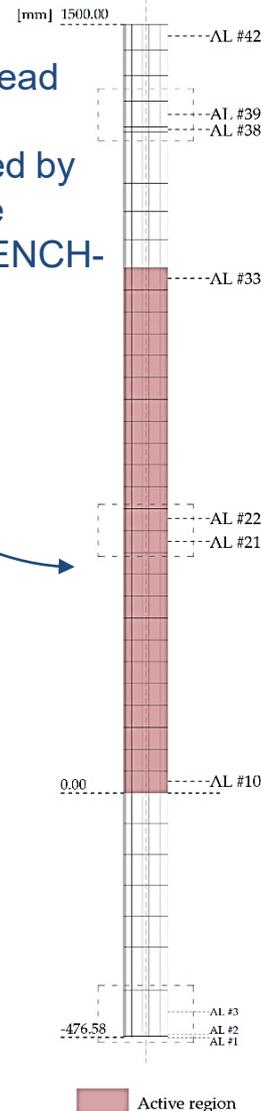
- **Ring 1:** unheated rod + grids
- **Ring 2:** 8 inner heated rods + grids
- **Ring 3:** 12 outer heated rods + grids
- **Ring 4:** 4 corner rods + grids + shroud



Ring	Radius
Ring #1	6 mm
Ring #2	27.975 mm
Ring #3	39 mm
Ring #4	42.38 mm

AXIAL NODALIZATION

- **Axial level 1:** lower head (dummy)
- **Axial level 2:** occupied by core supporting plate
- **Axial level 3-42:** QUENCH-06 test bundle



QUENCH-06 COR NODALIZATION (2)

COR type: PWR

Core radius = 0.04238 m → shroud outer radius

Vessel radius = 0.039 m → R_3 of COR nodalization

Vessel thickness = 0.00238 m → shroud thickness

Flat transition vessel-lower head

Lower elevation of COR support plate = - 0.4742 m

Thickness of COR supporting plate = 0.0042 m → equal to grid thickness

Cladding: all rods cladding, corner rods.

ZrO₂ Pellets: supporting ZrO₂ structures (ring: 1,2,3).

Grids: supporting (SS, Zry) structures + supporting core grid (COR_PLATE) in axial level 2.

Fuel: ELHEAT option on (ring: 2,3)

Shroud: SH component

- W as MATHT
- Mo as ELM1
- Cu as ELM2

In ELPOW voltages, outer resistance (~0.5mΩ/ring, variable in time) and electric power supplied to each heated ring are inserted.

In ELMAT resistivity options DEFW, DEFMO and DEFCU are turned on.

QUENCH-06 COR NODALIZATION (3)

!	fcnc1	fsscn	fcelr	fcela	flpup			
COR_RF	0.25	0.25	1.0	0.1	0.25			
!	ntpcor	rntpcor	icfgap	icffis				
COR_TP	NO	NO	NO	NO				
!	zr	zx	uo	ss	sx	cp		
COR_CHT	7500.0	7500.0	7500.0	2500.0	2500.0	2500.0		
!	ieumod	ihsdt	idtdz	icorcv				
COR_MS	INACTIVE	REQ	CVH	NOCONS				
!	mtuozr	mtzxzr	mtsxss	mtcpss	fuozr	fzxzr	fsxss	fcpsc
COR_CMT	1	1	2	2	0.2	0.0	1.0	0.0
!	drclmn	drssmn						
COR_CCT	1.0E-5	0.0						
!	size							
COR_SS	7	ln	ia	ir	issmod	issfai	tssfai	ssmetal
		1	2	1-4	PLATEG	TSFAIL	2400.0	STEEL
		2	10	1	PLATEG	TSFAIL	2400.0	STEEL
		3	6	2-3	PLATEG	TSFAIL	2400.0	STEEL
		4	11	2-3	PLATEG	TSFAIL	2400.0	ZIRC
		5	22	2-3	PLATEG	TSFAIL	2400.0	ZIRC
		6	34	2-3	PLATEG	TSFAIL	2400.0	ZIRC
		7	41	2-3	PLATEG	TSFAIL	2400.0	ZIRC

Best estimated through sensitivity analysis. They tune radial heat exchange

- No critical stainless steel structure diameter
- Critical diameter for Zry structures has been lowered

COR supporting plate
 Structure to support the Zirconia stack in the dummy rod (lower elevation 0 mm)
 Inconel lower grid → modeled as stainless steel
 Zry spacer grids placed at different altitudes

QUENCH-06 COR NODALIZATION (4)

```
!
COR_LP      2      iaxsup      hdbh2o      ppfail      vfall      ntlp
!           100.0      2.0E7      1.0E-5      1
COR_LH      6      nlnh      nlnslh
!           0
COR_LHD     5      nlnht      nlnhta
!           4
! is      tlnh      radlnh      icvcav      ihscav      hsside      vflhhs      icfelh      icfelhs      icfcnv
1 300.0    6.0E-3    'CONTAINMENT'
2 300.0    0.027975  'CONTAINMENT'
3 300.0    0.039     'CONTAINMENT'
4 300.0    0.04238  'CONTAINMENT'
5 300.0    0.04238  'CONTAINMENT'
!
COR_LHF     hdbpn      hdblnh      mdhmpo      ihmpmlh      tpfail      cdispn
!           100.0    1.0E6      MODEL      MODEL      9999.0     1.0
COR_SHM     shmat
!           SS
COR_MAT     1 ! cormat      matnam
!           1 SS      ZIRCALOY
```

Stainless steel in COR description has been modified and substituted with Zircaloy. Mandatory operation since **it is not possible to define SH component made directly as Zircaloy**

Lower head default properties has been kept.

In this way also Supporting Structures are altered.

Not a big concern..

QUENCH-06 HS NODALIZATION

In the HS package thermal insulation system is modeled.

Heat structures [1-42] have:

- LHS: *CalcCoefHS* option with the relative CV/Bypass + enabled radiation option

- $\varepsilon_{Zry} = 0.8, \varepsilon_{SS} = 0.07$
- Rad.Path* = *Bypass thickness*,
- Heated diameter* = 0.001 m].

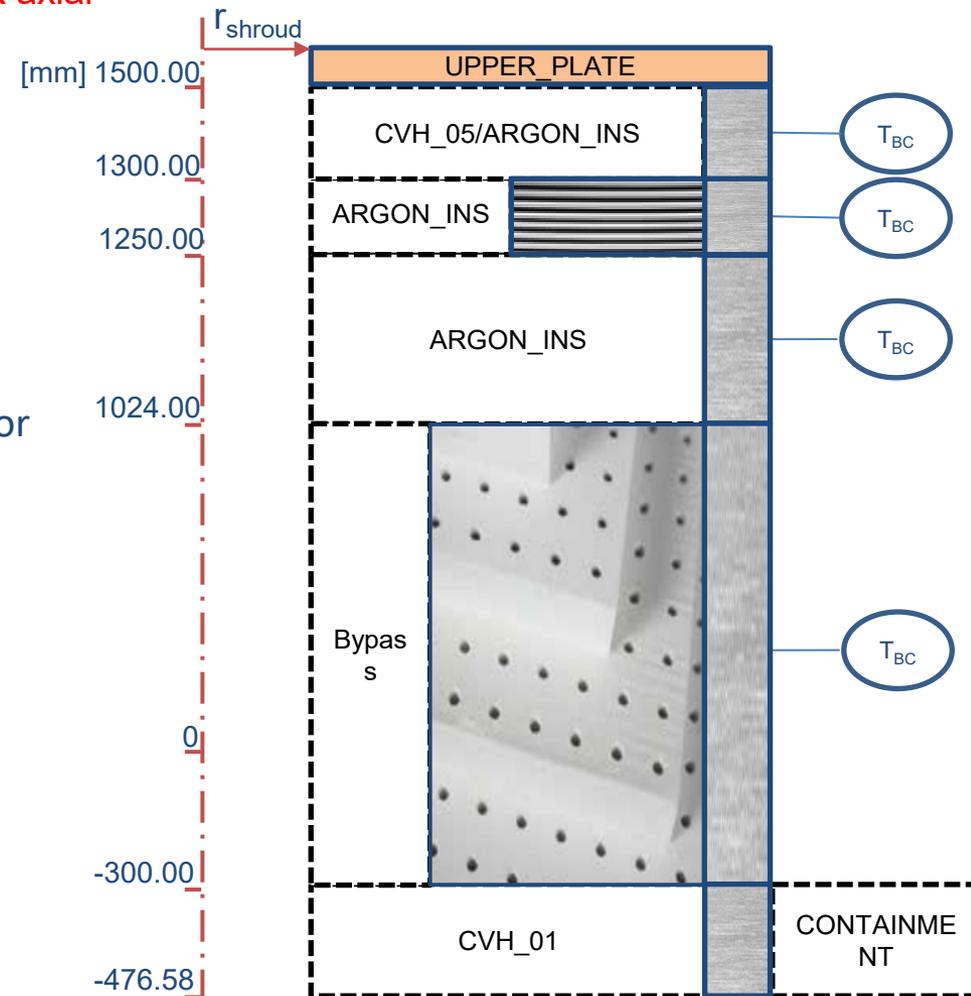
- RHS: boundary *TempCF* (from experimental data or reasonably guessed) or *CalcCoefHS* with CONTAINMENT.

Heat structure [43] UPPER_PLATE for the upper thermal shield.

Heat structure materials:



Cylindrical geometry



QUENCH-06 SENSITIVITY COEFFICIENTS

Some sensitivity coefficients have been modified to better describe specific phenomenologies, unusual geometry and to solve some numeric issues arising from the fine nodalization of the input.

CVH_SC:

1. 4415(2) = 1.0E-5
2. 4415(3) = 1000.

One of the most occurring errors was

ERROR IN CVHMOM: ERROR SOLVING MATRIX IN SPARSE FORM

Hence with those modifications, error tolerance is enhanced and an higher n° of allowed iterations per cycle are permitted.

HS_SC:

1. 4205(1) = 1.0E-5 [kg]

This SC refers to the minimum mass of unmelted steel on which an HS could still run without being deactivated.

This attempts was devoted to preventing the following error:

UPPEST 4 HS BEING DEACTIVATED (made just by a thin slab of steel).

COR_SC:

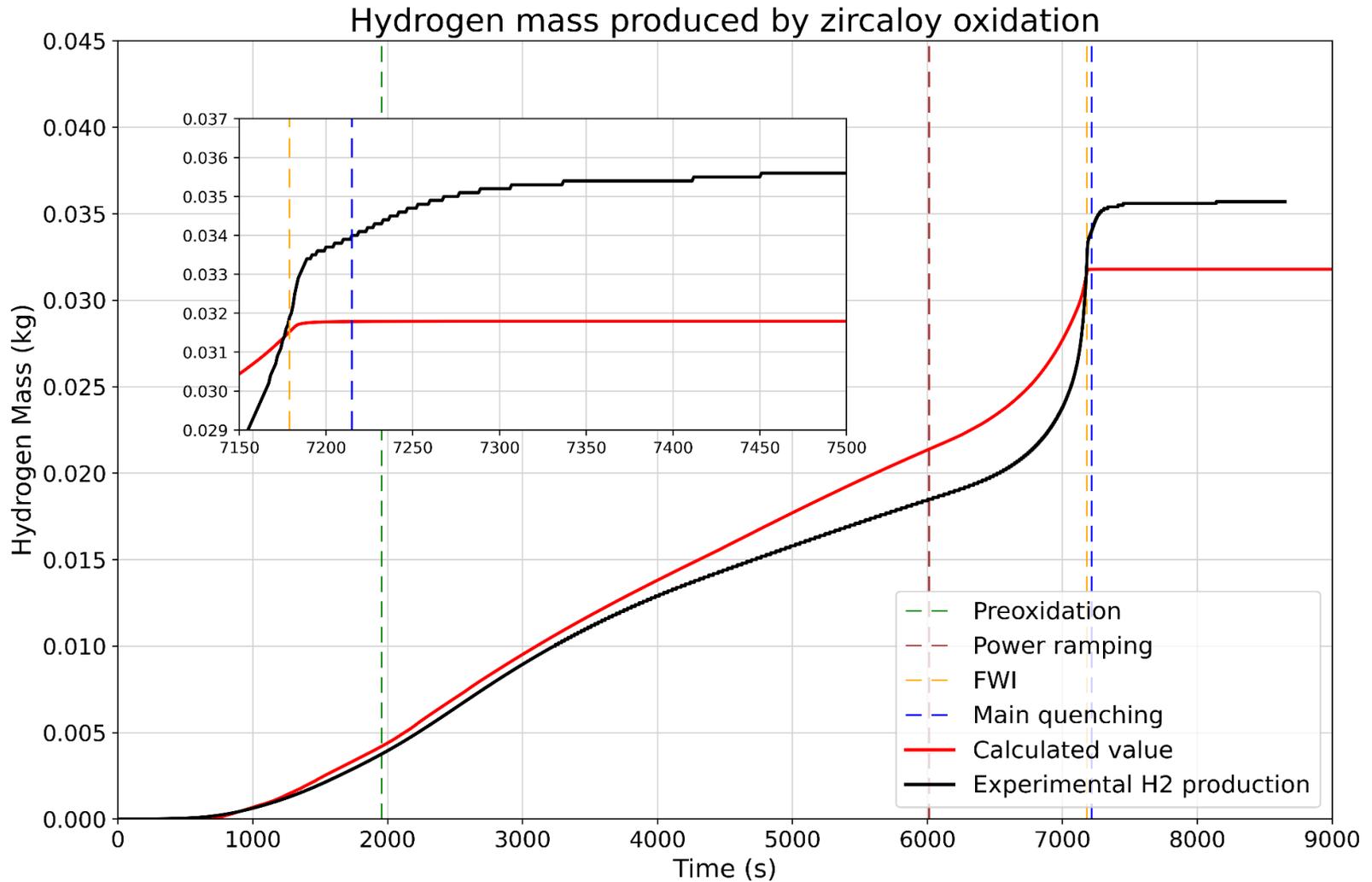
1. 1004(1) = 1100 [K] default
2. 1132(1) = 2990.0 [K]
3. 1132(2) = 3695 [K]
4. 1502(1) = 1.0E-9 [kg]
5. 1502(2) = 1.0E-7 [kg]

Some SC are needed while dealing with so light-weight component

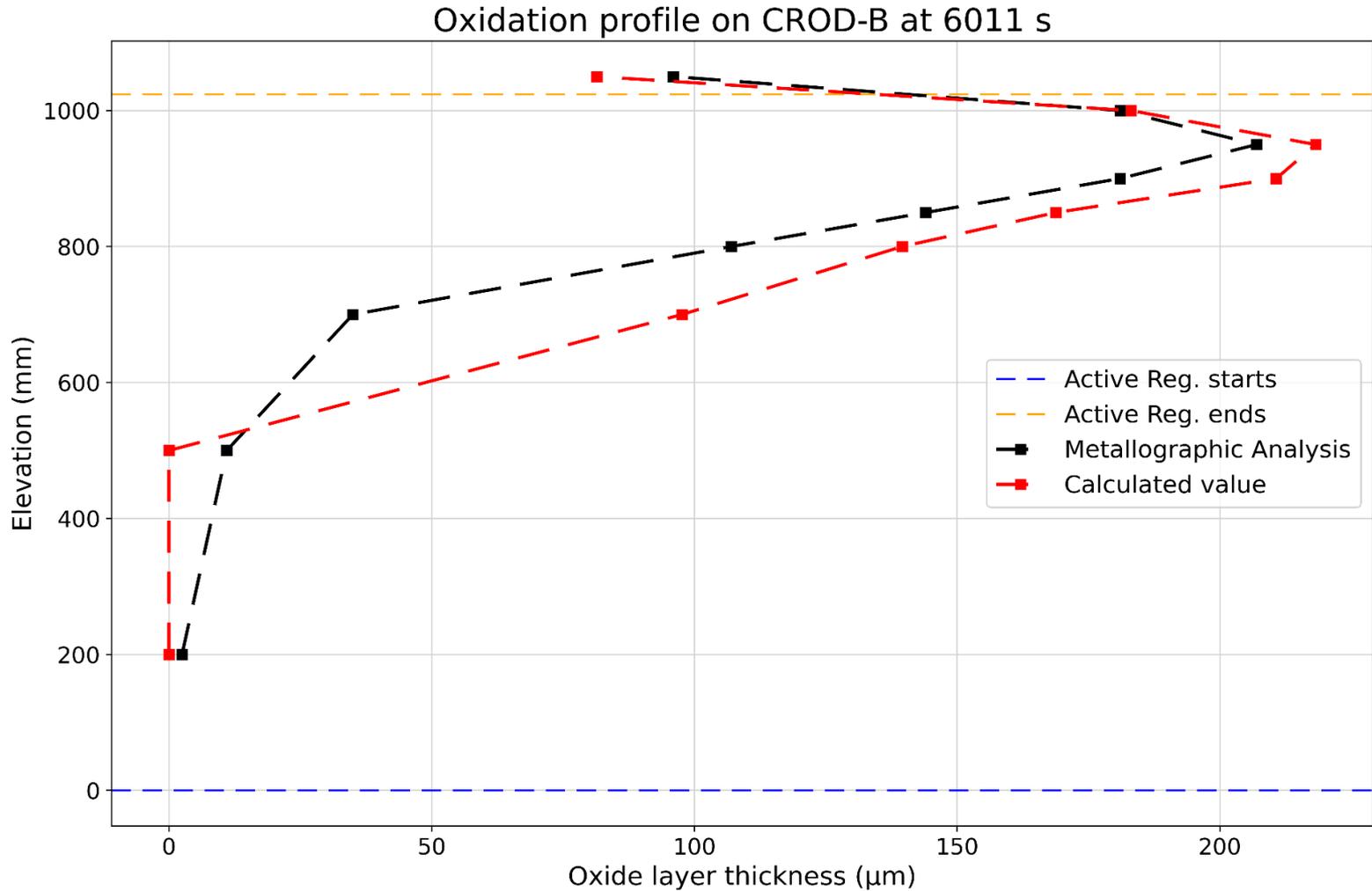
COR_SC 1401 instead is devoted to control the DT(COR).

REFERENCE CASE RESULTS AND COMPARISON WITH EXPERIMENTAL DATA

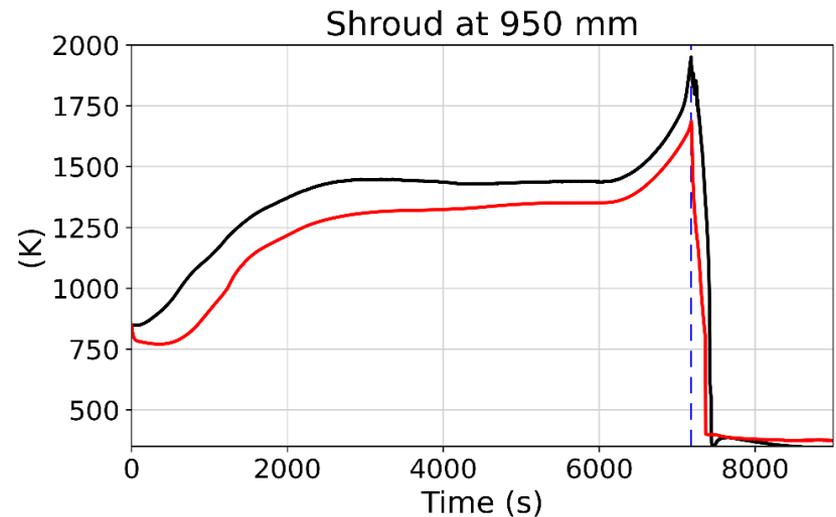
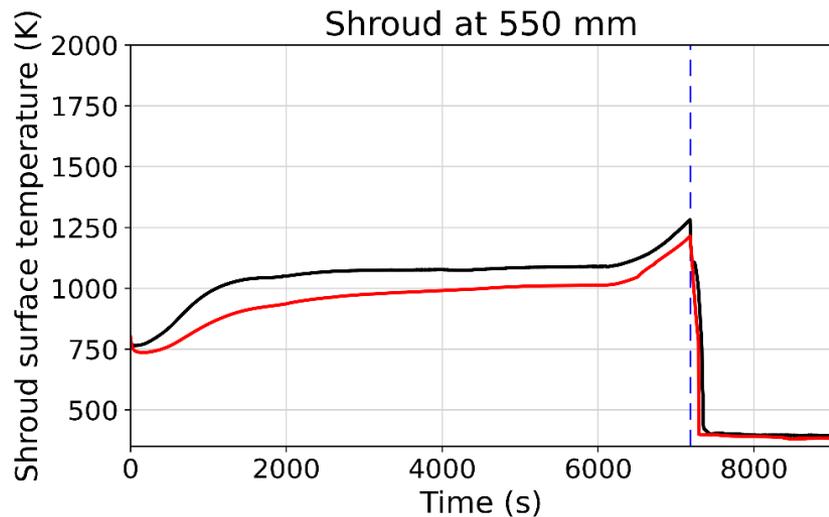
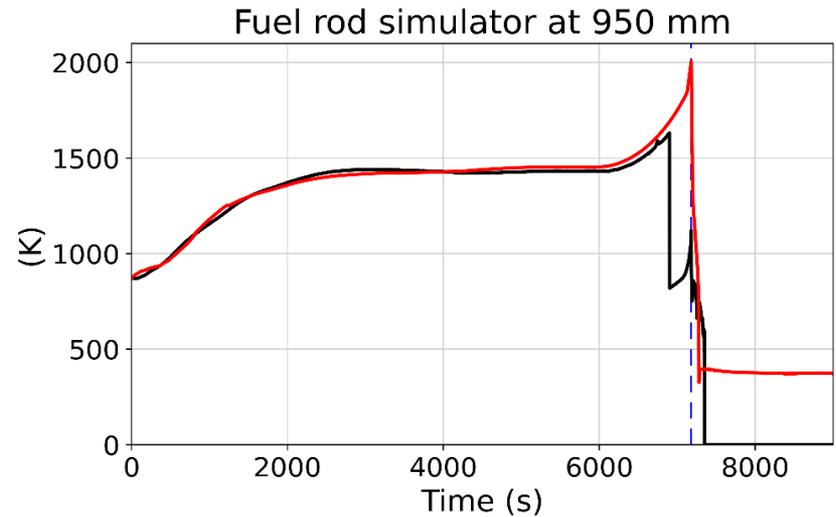
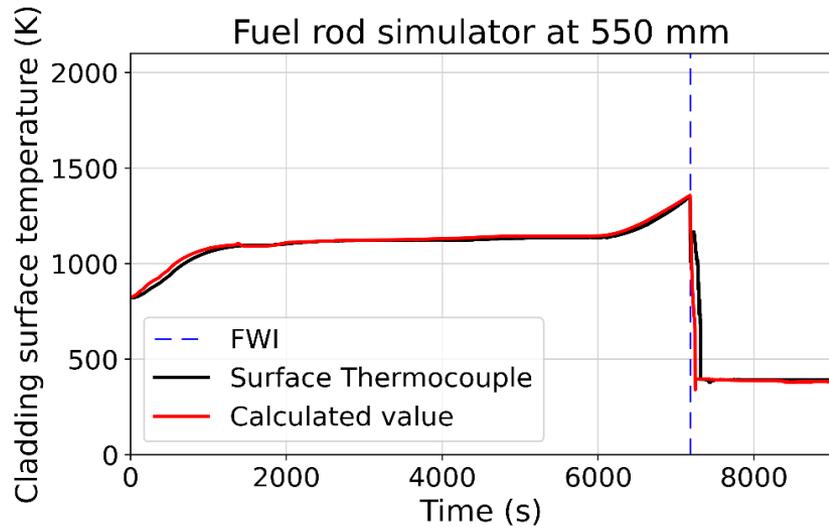
RESULTS



RESULTS



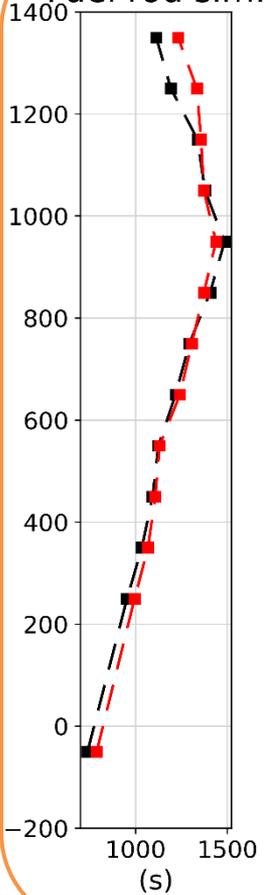
RESULTS



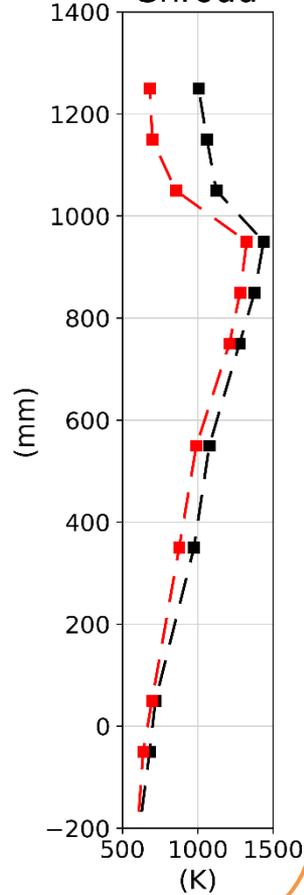
RESULTS

— Surface thermocouple
 - - Calculated trends

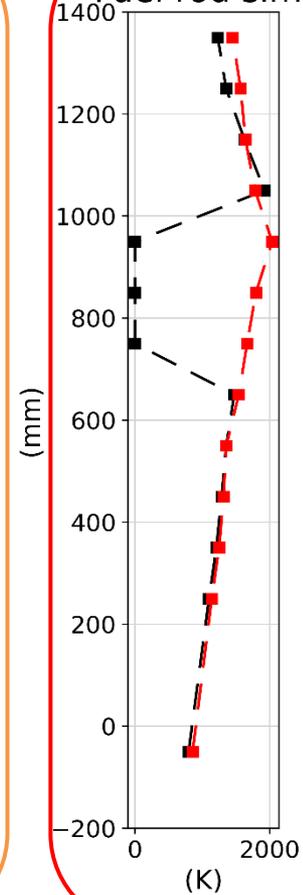
Fuel rod sim.



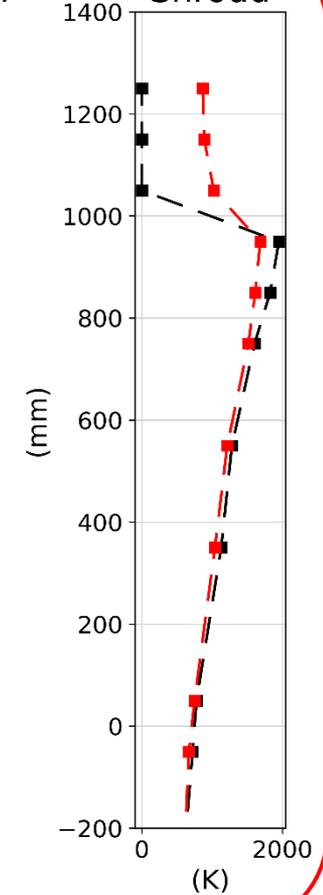
Shroud



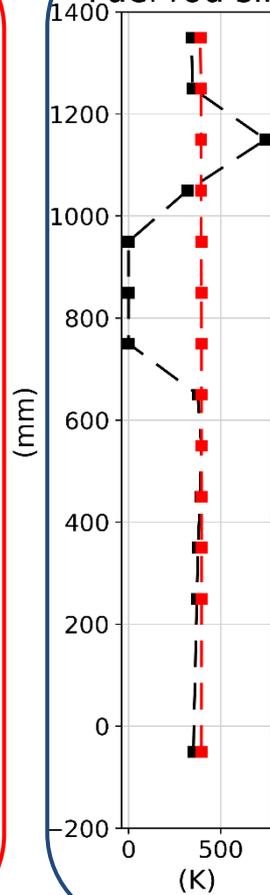
Fuel rod sim.



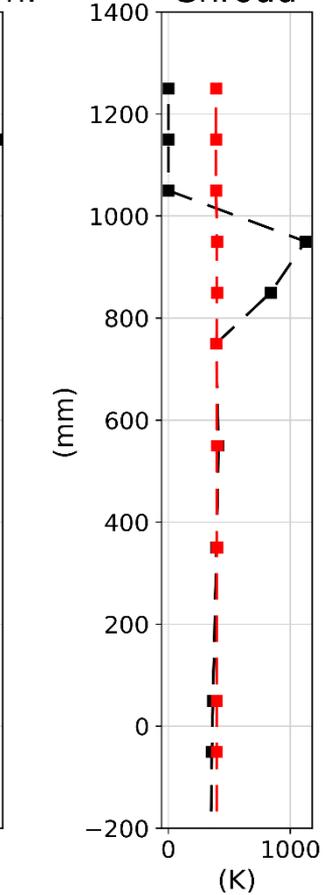
Shroud



Fuel rod sim.



Shroud



Preoxidation
 $t = 4000 \text{ s}$

Power ramping
 $t = 7179 \text{ s}$

Quenching
 $t = 7400 \text{ s}$

RESULTS

[Fast Fourier Based Transform Method](#) (FFBTM) tool delivers in output a **dimensionless indicator AA** for each variable in each phenomenological windows that acts as **indicator of the quantitative accuracy of the code results**.

Variables	Preoxidation	Power ramping	Quench and rest
Hydrogen Prod.	0,15	0,20	0,23
Rod Temperature 950 mm	0,03	-	-
Shroud Temperature 950 mm	0,13	0,14	0,33
Rod Temperature 1250 mm	0,31	0,21	0,73
Shroud Temperature 1250 mm	0,57	-	-
Rod Temperature 50 mm	0,21	0,21	0,80
Rod Temperature 550 mm	0,03	0,02	0,49
Collapsed Liquid level	0,14	0,07	0,94

- $AA \leq 0.3$: very good code prediction;
- $0.3 < AA \leq 0.5$: good code prediction;
- $0.5 < AA \leq 0.7$: poor code prediction;
- $0.7 < AA$: insufficient.

Issues:

1. [Elevation 1250 mm](#) is critical in the input.
2. Difficult to catch [evaporation after FWI](#) at 50 mm and 550 mm (affecting Liquid Level).

INPUT ISSUES

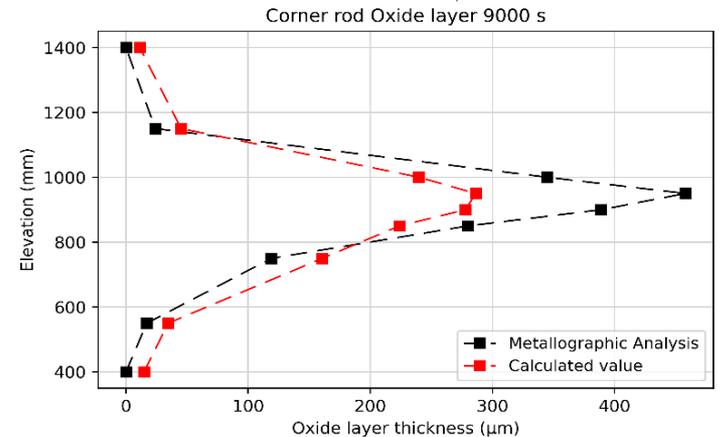
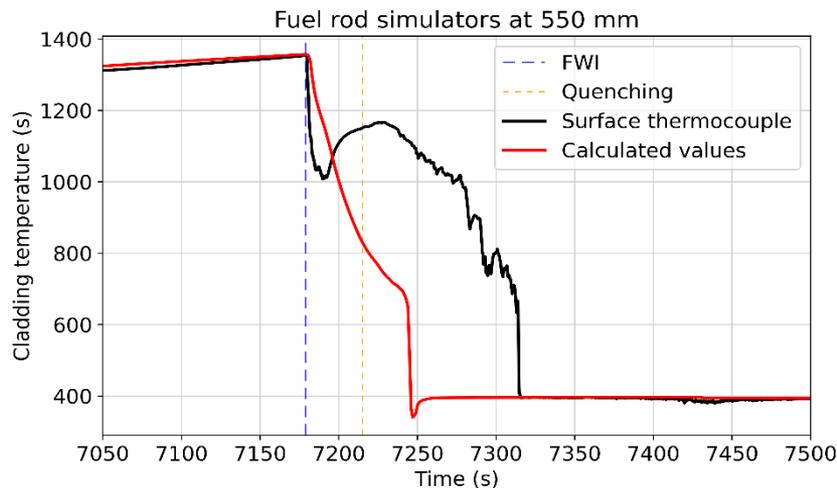
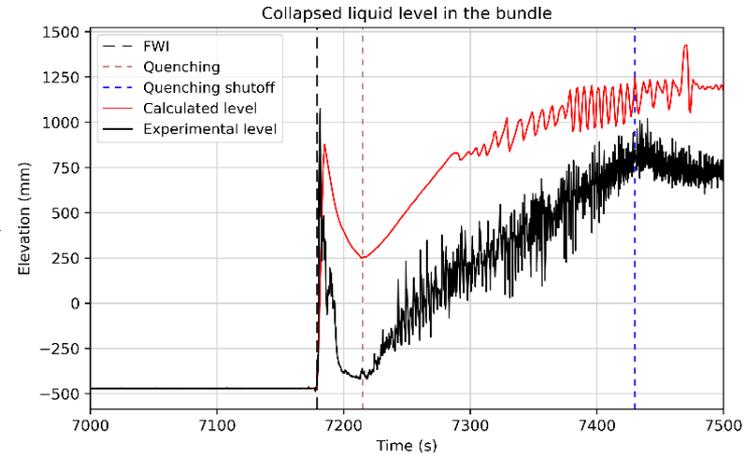
Reference Input does not predict evaporation of FWI water

Waterfront is located at higher altitude

Rod temperature does not increase again in between the two quenching

No further 4 g of H₂ generation

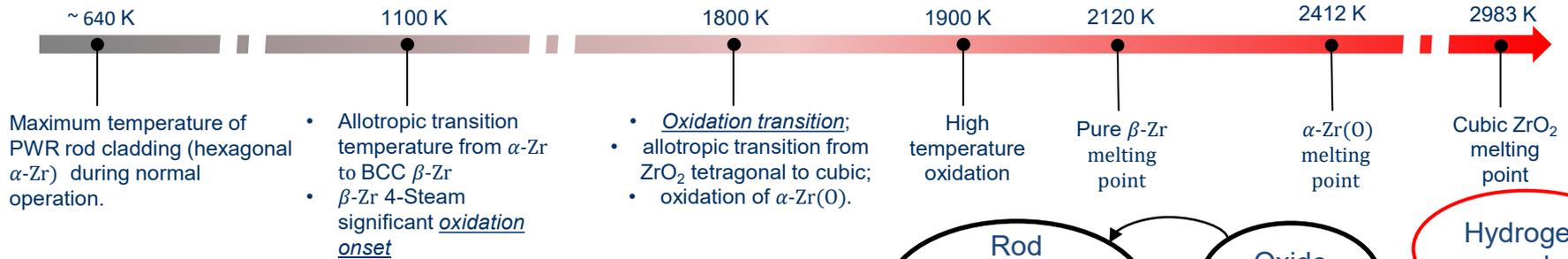
Final oxide thickness is underestimated



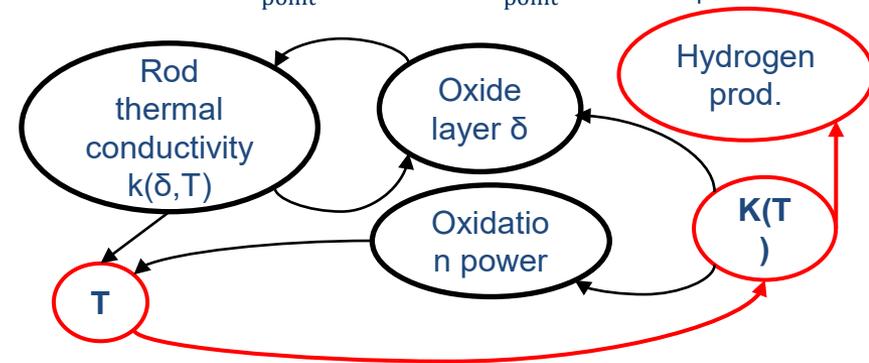
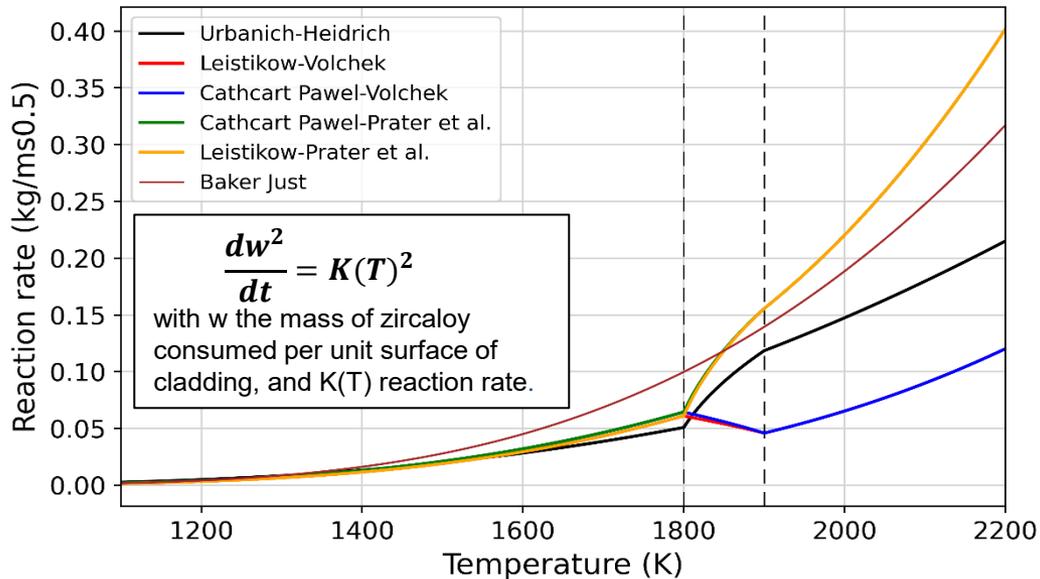
SENSITIVITY ANALYSIS ADOPTING DIFFERENT ZIRCALOY-STEAM OXIDATION CORRELATIONS

ZIRCALOY-STEAM OXIDATION

Zry oxidation kinetics



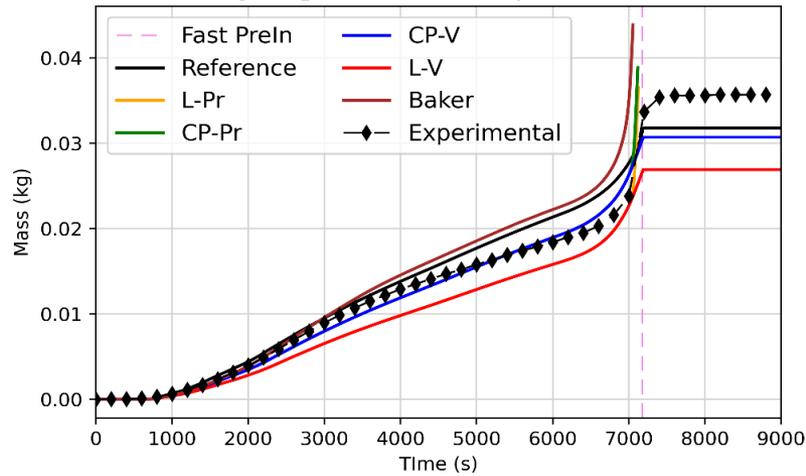
Correlations on K(T)



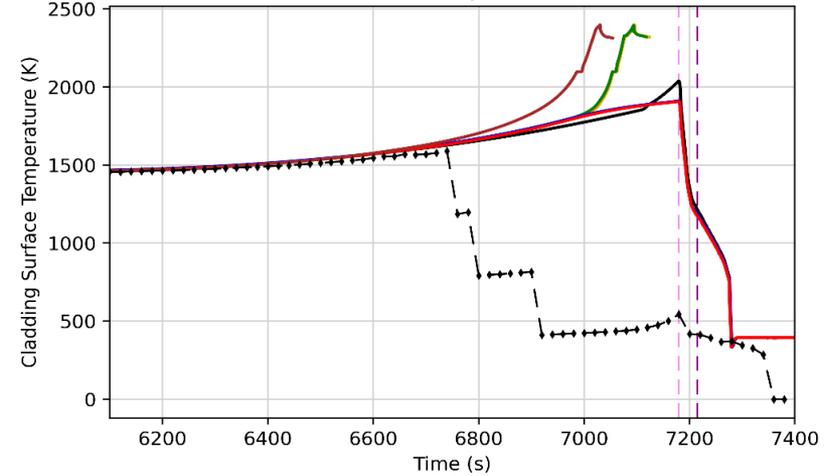
Simulations	K(T) T: [1100 K-1800 K]	K(T) T > 1900 K
1. Reference	Urbanich-Heidrich (default)	
2. Baker	Baker-Just	
3. L-V	Leistikow-Schanz	Volchek [1]
4. CP-V	Cathcart-Pawel	Volchek [1]
5. L-Pr	Leistikow-Schanz	Prater-Courtright
6. CP-Pr	Cathcart-Pawel	Prater-Courtright

SA RESULTS

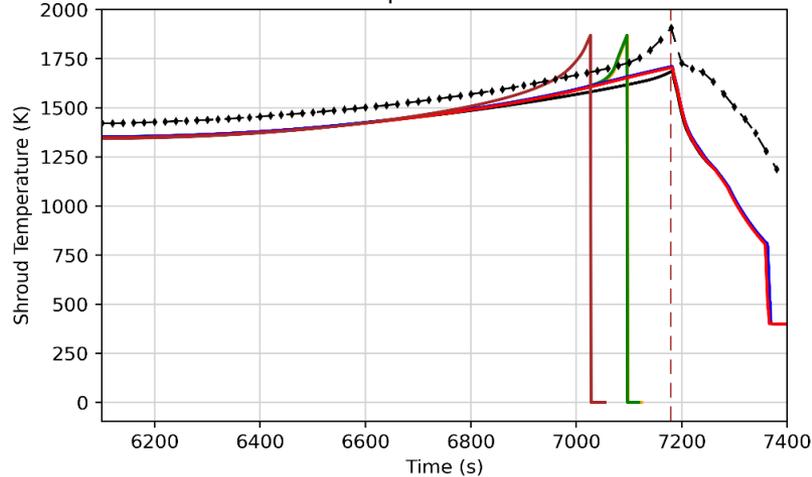
Hydrogen cumulative production



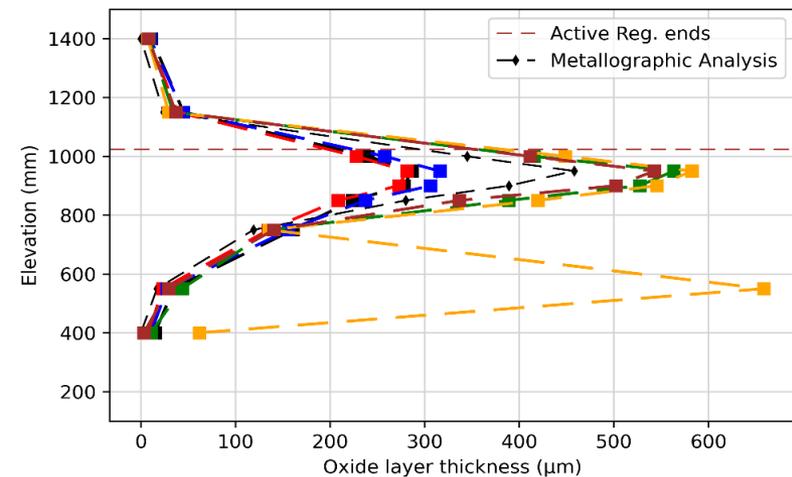
Fuel rod simulator temperature at 950 mm



Shroud temperature at 950 mm



Corner Rod A oxide thickness at 9000 s

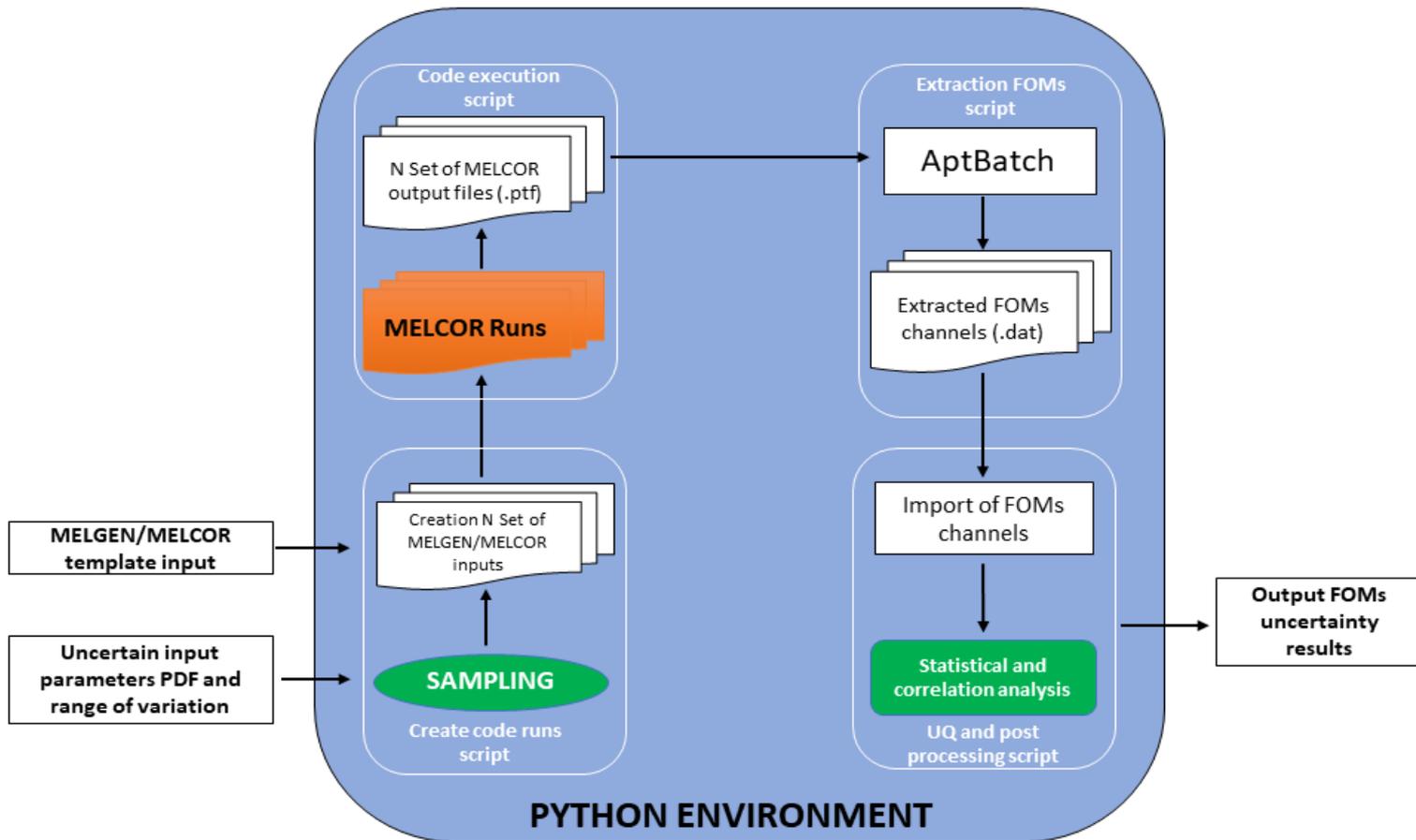


UNCERTAINTY ANALYSIS ADOPTING INPUT WITH CATHCART-PAWEL & VOLCHEK OXIDATION CORRELATIONS

UA TOOL

- The probabilistic method to propagate input uncertainty has been chosen to conduct the Uncertainty Analysis (UA).
- A tool in Python has been developed to conduct the UA. The Uncertainty Tool permits to set the UA in terms of uncertainty input parameters Probabilistic Density Functions (PDFs), sampling methods (e.g. Random Sampling, Latin Hypercube, etc.) and response data.
- The in-house tool, substitute the sampled uncertain input parameters in the sets of MELGEN/MELCOR inputs, run MELCOR simulations and extract the desired FOMs channels through the AptBatch executable.
- In this present UQ application, the **hydrogen cumulative mass production** has been selected as FOMs.
- Based on Wilks theory, a minimum of 59 code runs are required for one-sided confidence level of 95% in the case one FOM is selected.

UA WORKFLOW



UNCERTAINTY QUANTIFICATION HYPOTHESES (1)

- The uncertain input parameters, their ranges and PDFs have been provided by KIT leader of task 1 (QUENCH-06 experiment) of IAEA CRP I31033.

Name	Distribution Type	Mean	Parameters	
Steam_flow_rate, Argon_flow_rate, Quench_flow_rate [-]	Normal	1	low	0.98
			up	1.02
			St.dev	0.0133
Steam_temperature, Argon_temperature, Quench_temperature[-]	Normal	1	low	0.98
			up	1.02
			St.dev	0.0133
Outler_pressure [bar]	Normal	2E5	low	1.8E5
			up	2.1E5
			St.dev	1E4
FWI_pressure [bar]	Normal	6E5	low	5.7E5
			up	6.3E5
			St.dev	2E4
FWI_area [m ²]	Uniform	9.9E-5	min	8.91E-5
			max	1.09E-4
FWI_Friction [-]	Uniform	11	min	7.7
			max	14.3
Res_In, Res_Out [-]	Uniform	1	min	0.85
			max	1.15
Radial_Factor [-]	Uniform	1	min	0.8
			max	1
Biot_HTC [W/m ² K]	Uniform	1.5E5	min	1E5
			max	2E5
Max_Wall_Superheating [K]	Uniform	600	min	500
			max	700

Out of bundle wire R
F_{celr} coeff.
For the QUENCH Model

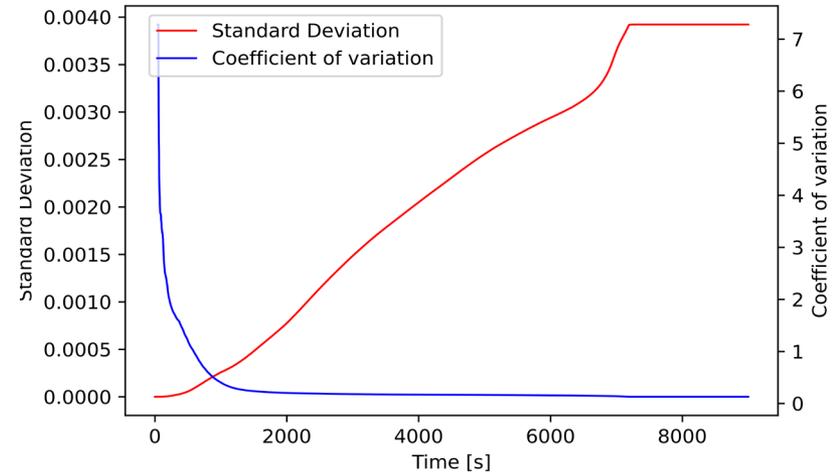
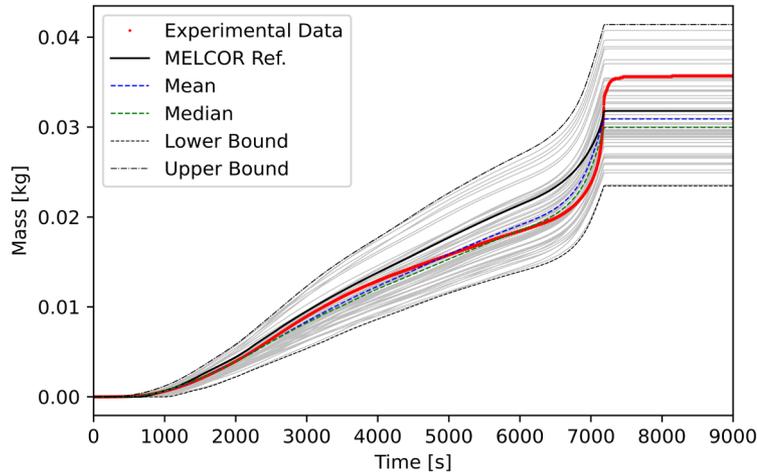
UNCERTAINY QUANTIFICATION HYPOTHESES (2)

- In addition, also the oxidation onset temperature and the parameters of the Arrhenius formulation of the Zircaloy-Steam reaction rates (regarding both Cathcart-Pawel and Volchek formalisms) have been varied.

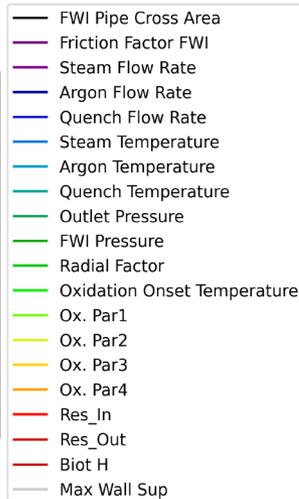
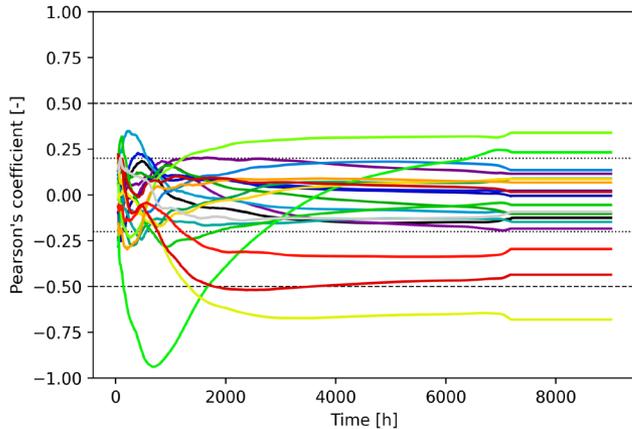
Name	Distribution Type	Mean	Parameters	
Onset_Ox_Temperature [K]	Uniform	1100	low	900
			up	1200
Ox. Par1 [K]	Normal	294.2	low	256.54
			up	331.85
			St.dev	25.1
Ox.Par2 [J]	Normal	20100	low	19768.35
			up	20431.65
			St.dev	221.1
Ox. Par3 [K]	Normal	107.4	low	102.03
			up	112.77
			St.dev	3.58
Ox.Par4 [J]	Normal	26822.2	low	26607.62
			up	27036.77
			St.dev	143.05

UA RESULTS

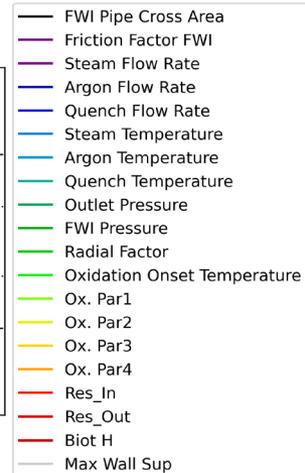
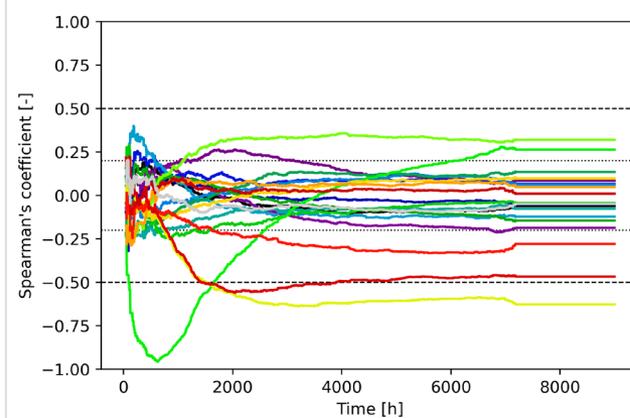
Hydrogen Production



Pearson Coefficient

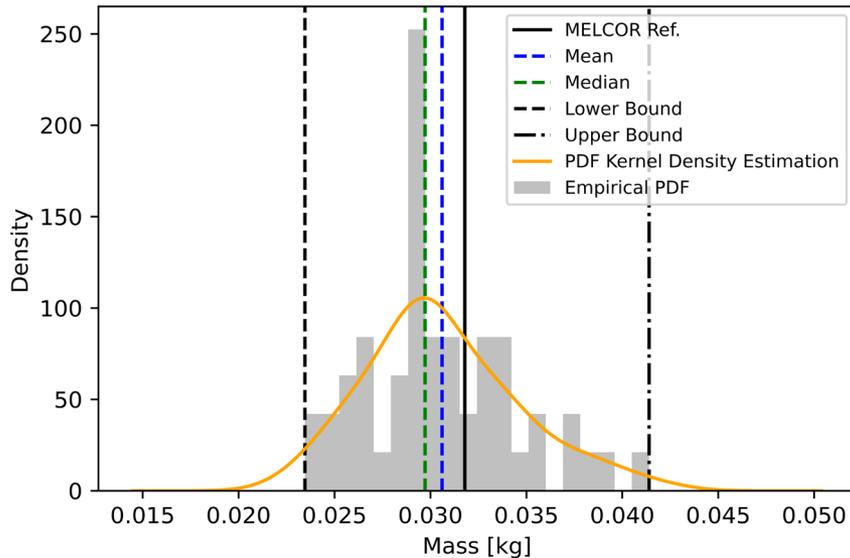


Spearman Coefficient



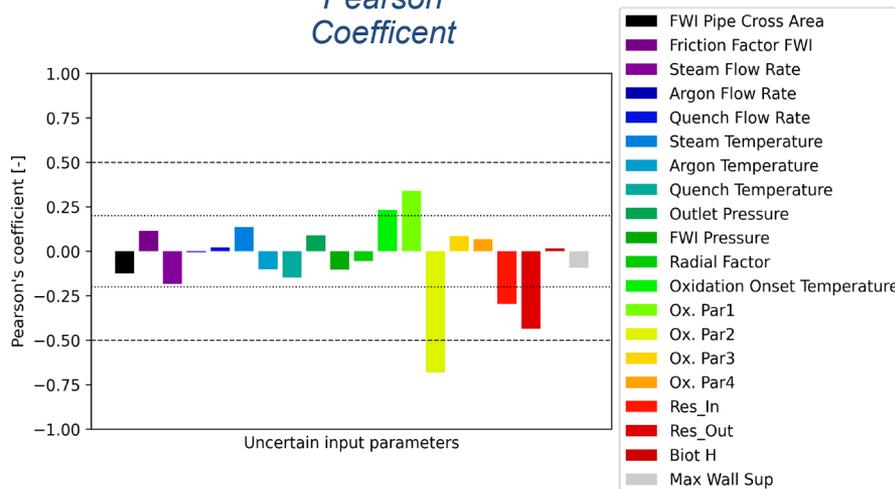
UA SCALAR ANALYSIS ON THE FINAL AND MAXIMUM VALUE OF THE FOM

Estimated Hydrogen production pdf

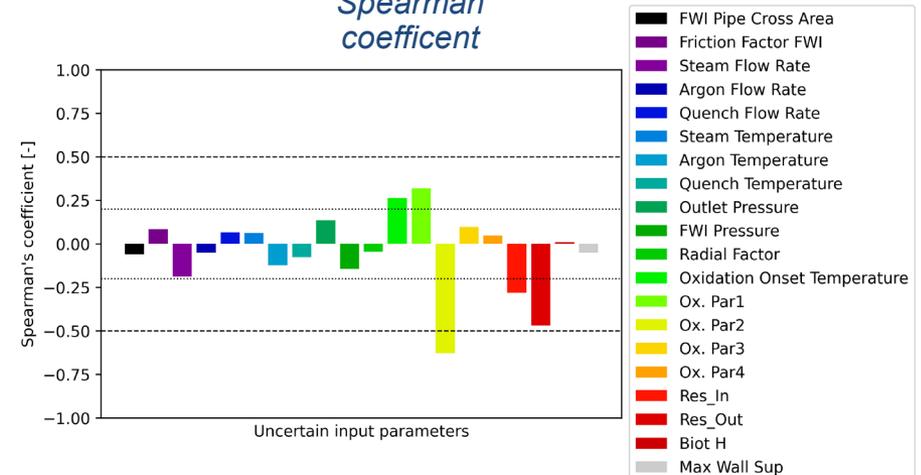


Uncertainty outcome	
Mean FOM	0,0306 kg
Median FOM	0,0297 kg
Lower Bound FOM	0,0235 kg
Upper Bound FOM	0,00414 kg

Pearson Coefficient



Spearman coefficient



UA REMARKS

The parameters with higher correlation with the FOM are:

- **Oxidation onset temperature:** as expected, by lowering it, the hydrogen mass predicted by the simulation increases;
- **Oxidation parameters 1 & 2:** they define the Arrhenius type reaction rate of *Cathcart-Pawel correlation* for the zircaloy oxidation when zircaloy structures temperature is under 1800 K.

$$K(T) = Ox.Par1 * e^{-\left(\frac{Ox.Par2}{RT}\right)}$$

- **Res_In** and **Res_Out:** they model the out-of-bundle wire resistances for the two rings of heated rods.

Standard deviation of the final distribution of the FOM is 12% of the mean value.

CONCLUSIONS

QUENCH-06 nodalization may be employed, just modifying the boundary conditions, in every QUENCH test where fuel rod simulators are sheathed by zircaloy cladding.

QUENCH-06 *Reference Input*:

- Ability to reproduce the main phenomenologies occurring during **preoxidation** and **power ramping** phases
 - hydrogen build up and oxidation are in agreement with the experimental trend;
 - temperature reconstruction matches closely the experimental evolution.
- During **quenching**, it does not reproduce FWI evaporation:
 - no further hydrogen production and no thickening of oxide layers;
 - collapsed liquid level is overestimated.

Sensitivity analysis has provided interesting insights:

- The **CP-V** simulation (Cathcart-Pawel and Volchek oxidation correlations) is suggested for future calculations;
- Shroud is predicted to fail while adopting Baker and Prater at el. Correlations

Uncertainty analysis has provided interesting insights:

- The experimental data is comprised in the uncertainty band;
- The uncertain input parameters with higher correlation with the FOM are: oxidation onset temperature, Oxidation parameters 1 & 2, Res_In and Res_Out.

CONCLUSIONS

Thank you very much for your attention!

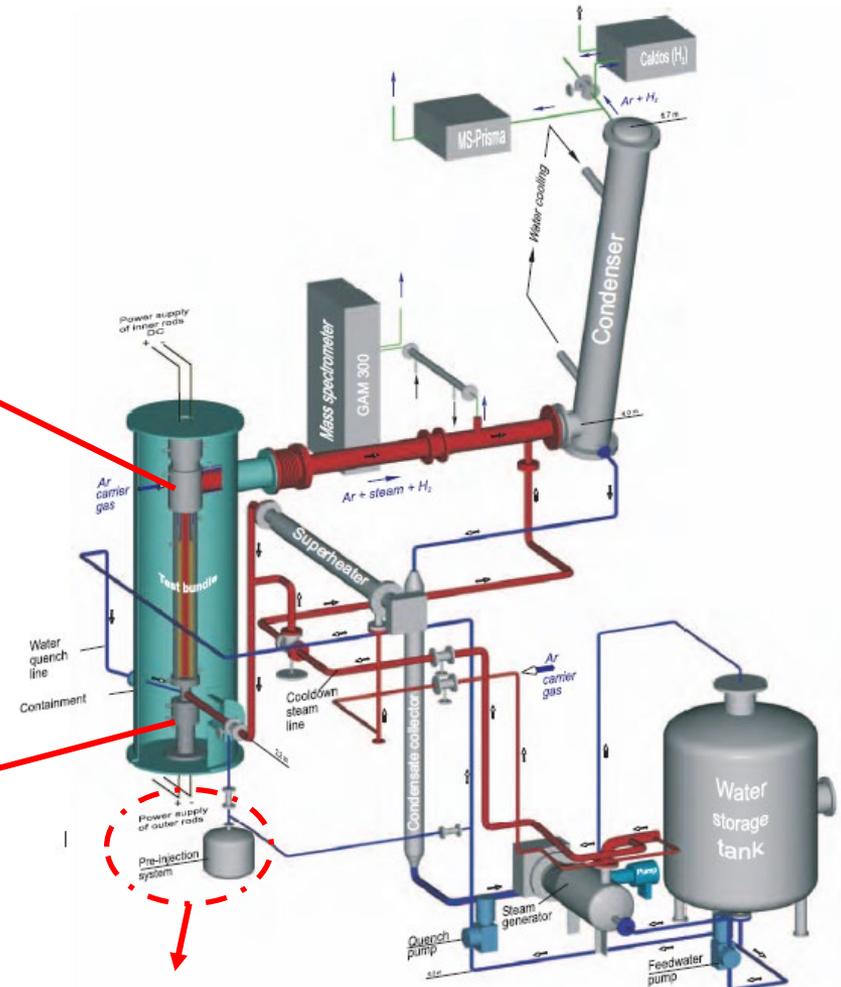
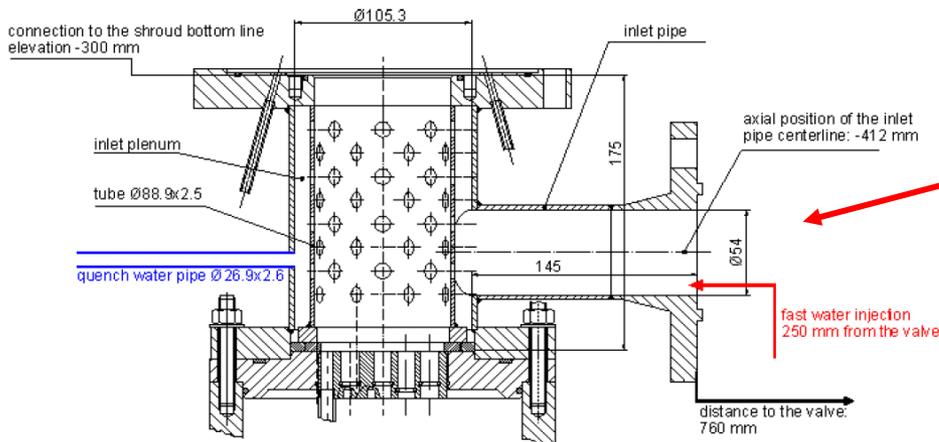
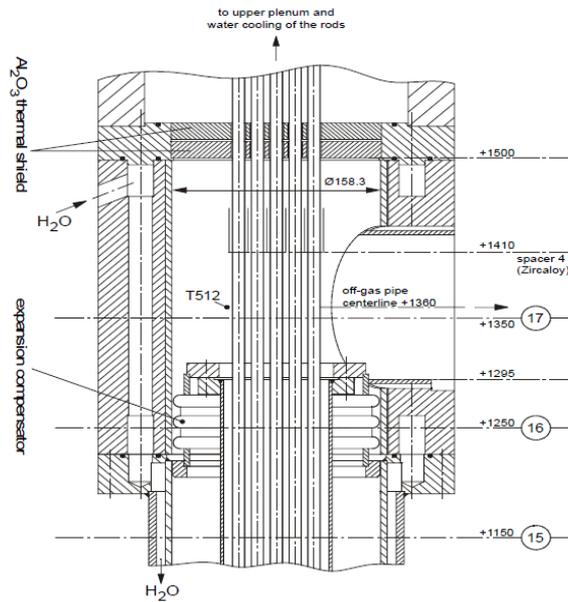
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REFERENCES

[1] A. Volchek, Y. Zvonarev e G. Schanz, «Advanced treatment of zircaloy cladding high-temperature oxidation in severe accident code calculations. Part II. best-fitted parabolic correlations,» *Nuclear Engineering and Design*, pp. 85-96, 2003.

APPENDIX I: WATER LOOP AND PLENA



Fast Water Injection system

APPENDIX II: SC QUENCH-06

Some SCs were added in order to solve timestep issues. In the following analyses, non mandatory parameters will be discarded.

Criteria for solving the Flow Eqts in Sparse Form [CVH]

- 4415(2): Convergence tolerance for iterative solver (Criteria for solving the Flow Eqts in Sparse Form)
- 4415(3): Max number of iterations permitted for the iterative solver

Stainless Steel Melting (Degassing) Parameters [HS]

- 4205(1): mass of unmelted steel below which the HS is deactivated and the remaining mass is relocated to the COR package

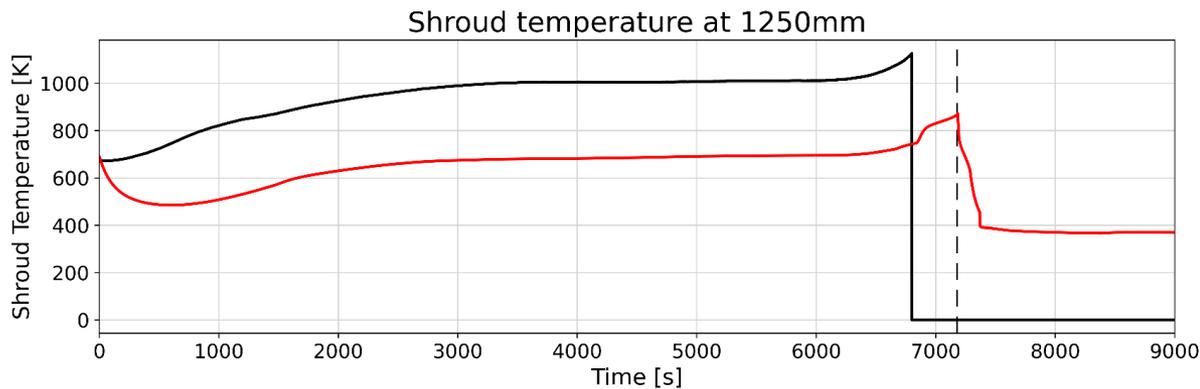
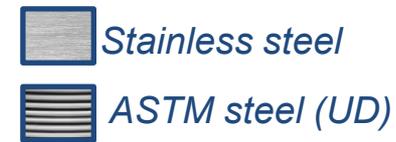
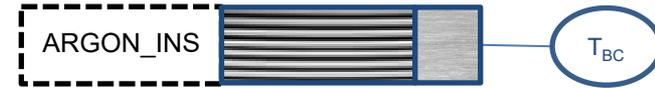
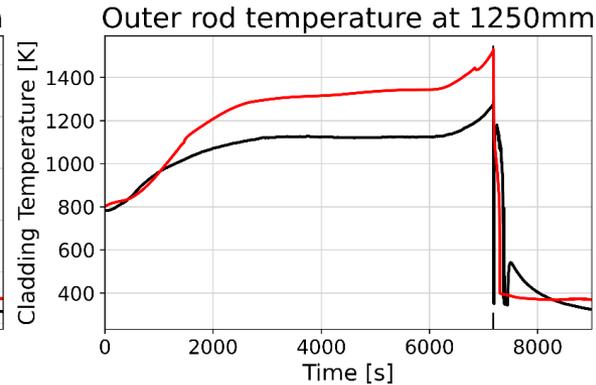
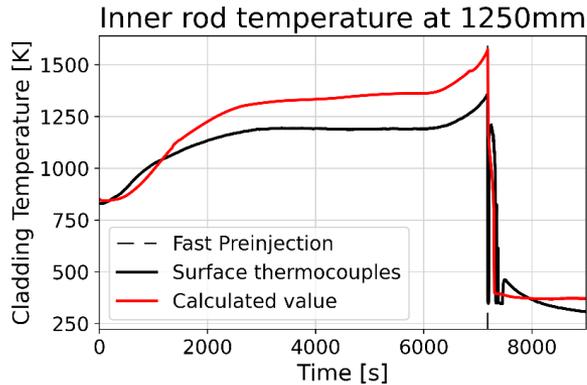
Core components failure parameters [COR]

- 1132(1): temperature to which oxidized fuel rods can stand in the absence of unoxidized Zr in cladding
- 1132(2): temperature at which fuel rods fail, regardless the composition of the cladding

Minimum Component Masses [COR]

- 1502(1): minimum total mass of a component
- 1502(2): minimum mass of a component subject to the max temperature change criterion for dt control

APPENDIX III: ELEVATION 1250 mm



Argon_Ins control volume and the heat structure (composed of the expansion compensator and the inner wall cooling jacket) are not correctly modeling radiative heat loss.