Karlsruhe Institute of Technology

ATF modelling in Severe Accident Codes

F. Gabrielli[1], T. Hollands[2], L. Lovasz[2], L. Carénini[3], D. Luxat[4] and J. Phillips[4]

[1] Karlsruhe Institute of Technology (KIT), [2] Gesellschaft für Anlagen- und Reaktorsicherheit (GRS) gGmbH

[3] Institut de Radioprotection et de Sûreté Nucléaire (IRSN), [4] Sandia National Laboratories (SNL)

Institute for Neutron Physics and Reactor Technology

Motivation

- ATFs have the potential for significant safety and performance improvements during normal/transient operations and severe accidents in Light Water Reactors.
- Much slower oxidation kinetics at high temperatures than the typical Zr-based alloy
  - → lower in-vessel H_2 build-up, lower energy generation, suppression of the H_2 explosions potential, Fission Product release reduction.

→ Enhancing the potential to activate/utilize accident management measures.

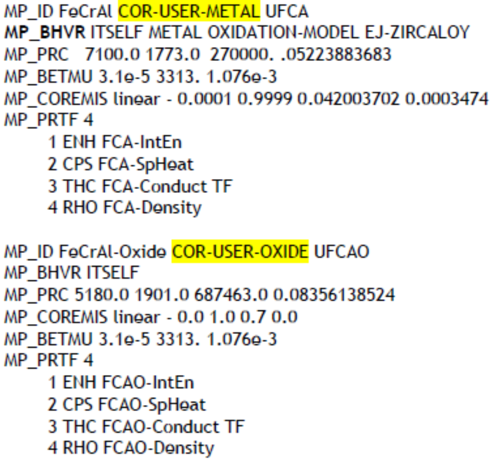
- Improvement of the severe accident codes capability to model ATFs is mandatory to enable the safety assessment of the innovative nuclear reactor concepts employing such materials.
- Extension of the modelling capabilities of AC^2/ATHLET-CD, ASTEC, and MELCOR is going on in the frame of the NEA QUENCH-ATF and IAEA CRP ATF-TS.
- In this phase, focus on FeCrAl and QUENCH-19 test.

Modeling New Materials in the SA Codes

- User usually employs the data stored in the available material database, i.e. for Zry/ZrO_2
  - Thermo-physical properties.
  - Oxidation models, i.e. Cathcart, Prater-Courtright, Urbanic, Best-fit,..
- The codes are flexible enough to introduce new materials either by adjusting the properties of a default material or to fully define behavior and properties by scratch.
- Current approach:
  - FeCrAl as a new material.
  - FeCrAl to be oxidizable.
  - FeCrAl/Oxide as the FeCrAl recipient oxide, whose properties defined based on the literature and on the feedback from the Quench experimental team.

MELCOR: Material Package (MP) Templating

- Material definition no longer requires a user to perform the two most common modification to materials.
    - Since core components only support certain material internally, users had to modify an existing material to alter properties, losing that material.
    - Create a wholly new material, which could only be used within the certain MELCOR packages such as the HS materials.
- It allows materials to assume a default material’s behaviors and properties.
- Four core package user defined materials (UDMs) now available within the database for every core component → enhancement of the user flexibility.



```
MP_ID FeCrAl COR-USER-METAL UFCA
MP_BHVR ITSELF METAL OXIDATION-MODEL EJ-ZIRCALOY
MP_PRC   7100.0 1773.0  270000. .05223883683
MP_BETMU 3.1e-5 3313. 1.076e-3
MP_COREMIS linear - 0.0001 0.9999 0.042003702 0.0003474
MP_PRTF 4
        1 ENH FCA-IntEn
        2 CPS FCA-SpHeat
        3 THC FCA-Conduct TF
        4 RHO FCA-Density

MP_ID FeCrAl-Oxide COR-USER-OXIDE UFCAO
MP_BHVR ITSELF
MP_PRC 5180.0 1901.0 687463.0 0.08356138524
MP_COREMIS linear - 0.0 1.0 0.7 0.0
MP_BETMU 3.1e-5 3313. 1.076e-3
MP_PRTF 4
        1 ENH FCAO-IntEn
        2 CPS FCAO-SpHeat
        3 THC FCAO-Conduct TF
        4 RHO FCAO-Density
```

J. Phillips, D. Luxat, 2020. MELCOR Modeling of QUENCH-15/19, Experts’ Meeting for the NEA joint undertaking QUENCH-ATF, OECD/NEA, Paris.
J. Phillips, 2020. Update on ATF Modeling: QUENCH-15/19, CSARP/MCAP Workshop.

ASTEC: Material Modeling

- User may define a new material in the input deck

```
STRU MDB
  STRU SET NAME 'Ar_cond'
    REF   "Properties of fictive material"
    TYPE  'MATERIAL'
    T_sol 5000.   T_liq 5001. M 1. ! always solid
    STRU PROPERTY NAME "rho_s(T)" LAW 'TABLE' VARIABLE 'T' SR1 VALUE  300.  2.0 2000.0 2.0  TERM END
    STRU PROPERTY NAME "lambda_s(T)" LAW 'TABLE'    VARIABLE 'T'
    SR1 VALUE  300.  0.2  800. 3.5  1060. 5. 1100 5. 1500. 10.0 2000. 20.0 TERM  END
    STRU PROPERTY NAME "h_s(T)" LAW 'TABLE` VARIABLE 'T'
    SR1 VALUE  300.  961.   900.  3.1D5 1500. 6.2D5  2000. 8.8D5 3000.  14.D5  4000. 19.D5  TERM END
    STRU PROPERTY NAME "em_s(T)" LAW 'TABLE` VARIABLE 'T' SR1 VALUE  300.  0.7 4000. 0.7  TERM END
  END
END
```

- or modifying the database

```
 HELP "m_O   (t+dt) = S ((m_O   (t)/S)**(1/model) + AGAIN EXP(-BGAIN/(R.T)) * dt )**model"
 HELP "e_O2Zr(t+dt) =   ((e_O2Zr(t))  **(1/model) + ATHIC EXP(-BTHIC/(R.T)) * dt )**model"
…..
STRUCTURE MODEL NAME 'BEST-FIT' LAW 'COEFF' VARIABLE 'T' VUNIT 'K' RUNLOW 0. RUNUPP 5000.
  SRG VALUE AGAIN 36.220D0 BGAIN 1.672D5 ATHIC 2.252D-6 BTHIC 1.502D5 MODEL 0.5 TERM
  X  1798.K
  SRG VALUE AGAIN 2.888D8 BGAIN 4.046D5 ATHIC 3.371D6 BTHIC 5.691D5 MODEL 0.5 TERM
  X  1900.K
  SRG VALUE AGAIN 2849.D0 BGAIN 2.23D5 ATHIC 0.008682D0 BTHIC 2.572D5 MODEL 0.5 TERM
 END
```

AC²/ATHLET-CD: FeCrAl Oxidation Model

- Assumption: Al oxidized only

$$Fe_xCr_yAl_z + z/2\cdot 3\ H2O \rightarrow Fe_xCr_yAl_{2z}O_{3z} + z/2\cdot 3\ H_2 + z\cdot\Delta h\ (\Delta h = 9.3\cdot 10^5\ J/mol)$$

- FeCrAl molar mass $M_{FeCrAl} = 99.3\cdot 10^{-3}$ kg/mol ($\Delta h = 9.36\cdot 10^6\ J/kg_{FeCrAl}$)

  $\rightarrow M_{Al2O3} = 102.0\cdot 10^{-3}$ kg/mol

- Oxidation Rate → Parabolic law derived from the analytical solution of the diffusion equation (as for Zr)

$$\mathbf{dW^2 = K(T)\cdot dt}\ (W: m_{O2}/A\ [kg/m^2],\ K: \text{reaction rate}\ [kg^2/m^4s],\ t: \text{time}\ [s])$$

- Reaction rate from the Arrhenius formulation

$$K = A\cdot e^{-B/(RT)} g(p_s)$$

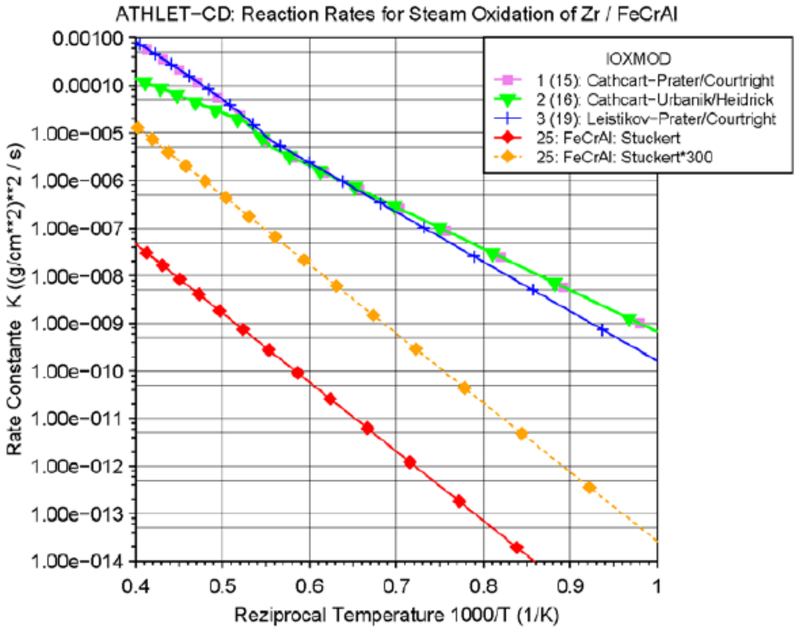
R=8.134 J/mol K, T: cladding Temperature [K], $g(p_s)$: reduction factor for steam starvation

A= 3.1 kg²/m⁴s, B= 2.78519 ·10⁵ J/mol (from KIT for one composition)

T. Hollands, 2020. Post-test analytical benchmarks–GRS simulation capabilities –, Experts' Meeting for the NEA joint undertaking QUENCH-ATF, OECD/NEA, Paris.

AC^2/ATHLET-CD: FeCrAl Oxidation Model

- $FeCrAl/Al_2O_3$ instead of Zry/ZrO_2 properties.
  - No temperature dependency considered
- Model 25 is based on a publication by Pint, et al., for KANTHAL APMT (69Fe+21.6Cr+4.9Al) and provided by KIT.
- Model 25 multiplied by 300 is derived from the ”State-of-the-Art Report on Light Water Reactor Accident-Tolerant Fuels“ of the OECD/NEA (NEA No. 7317).
- The new code version includes the possibility to implement additional correlations including enthalpy



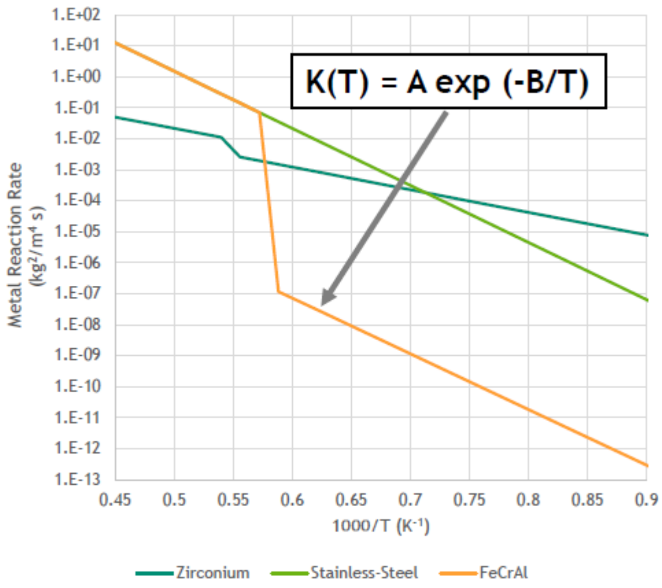
T. Hollands, 2020. Post-test analytical benchmarks–GRS simulation capabilities –, Experts’ Meeting for the NEA joint undertaking QUENCH-ATF, OECD/NEA, Paris.
Pint, B.A., et al., High Temperature Oxidation of Fuel Cladding Candidate Materials in Steam-Hydrogen Environments, Journal of Nuclear Materials 440, pp. 420-427, 2013.

MELCOR: FeCrAl Oxidation Model

- Based on prior work by INL/ORNL
- Reaction rates apply data from Pint, et.al., prior to breakaway.
  - Oxygen uptake data is converted to metal reacted and standard units.
  - Must assume prevailing oxides to convert from oxygen to metal reacted.

$$\mathrm{FE}+4/3\cdot \mathrm{H2O} \rightarrow 1/3\cdot \mathrm{Fe_3O_4}+4/3\cdot \mathrm{H2}$$
$$\mathrm{CR}+3/2\cdot \mathrm{H2O} \rightarrow 1/2\cdot \mathrm{Cr_2O_3}+3/2\cdot \mathrm{H2}$$
$$\mathrm{AL}+3/2\cdot \mathrm{H2O} \rightarrow 1/2\cdot \mathrm{AL_2O_3}+3/2\cdot \mathrm{H2}$$

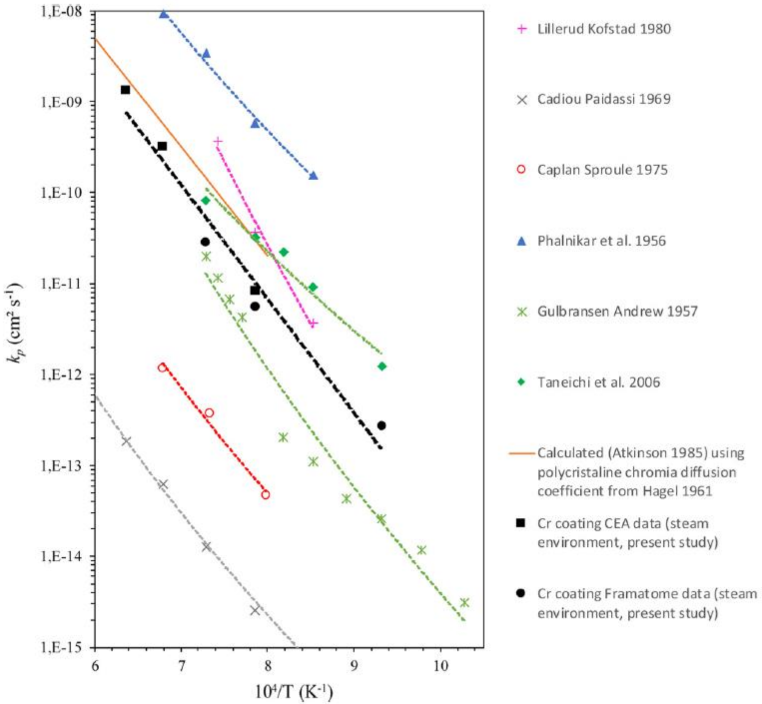
  - **$K=4360 \cdot e^{-(41376/T)}$**



- New MELCOR modeling allows specifying all the reaction parameters

Merrill, B.J., Bragg-Sitton, S.M., Humrickhouse, P.W., Modification of MELCOR for Severe Accident Analysis of Candidate Accident Tolerant Cladding Materials, NED 315 170-178. 2017.
Robb, K.R., Howell, H., and Ott, L.J., Design and Analysis of Oxidation Tests to Inform FeCrAl ATF Severe Accident Models, Oak Ridge National Laboratory, ORNL/SPR-2018/893 (July 2018).
Pint, B.A., et al., High Temperature Oxidation of Fuel Cladding Candidate Materials in Steam-Hydrogen Environments, Journal of Nuclear Materials 440, pp. 420-427, 2013.
Phillips, J., Luxat, D., 2020. MELCOR Modeling of QUENCH-15/19, Experts' Meeting for the NEA joint undertaking QUENCH-ATF, OECD/NEA, Paris.
Phillips, J., 2020. Update on ATF Modeling: QUENCH-15/19, CSARP/MCAP Workshop.

ASTEC: FeCrAl Oxidation Model



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

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

$$\boxed{\Delta m = 19.62 \cdot e^{-\frac{123783}{R \cdot T}} \cdot \sqrt{t}}$$

Brachet, J.-C., et al., 2020. High temperature steam oxidation of chromium-coated zirconium-based alloys: Kinetics and process, Corrosion Science 167 (2020) 108537.
Gabrielli, F., Sanchez-Espinoza, V.H., Wang, S. 2020. ASTEC modelling capabilities for analyzing the QUENCH-ATF tests, Experts' Meeting for the NEA joint undertaking QUENCH-ATF, OECD/NEA, Paris.

ASTEC: FeCrAl Oxidation Model

- Modifying the laws for oxygen mass gain and oxide thickness growth in the database relevant to the cladding steam oxidation.
- **Assumptions: 1) No temperature dependency considered 2) Δh of Zr employed.**

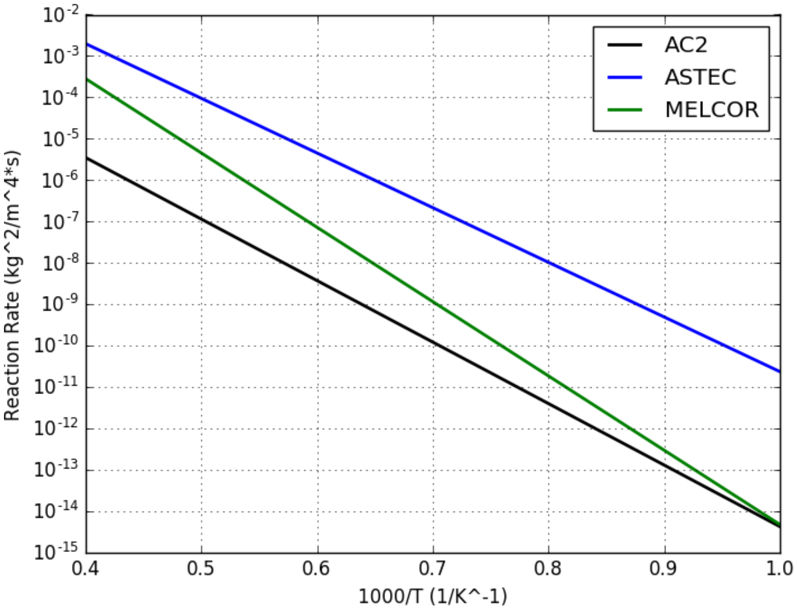
$$m_o(t+dt) = S.\left(\left(\frac{m_o(t)}{S}\right)^{\frac{1}{model}} + AGAIN.e^{\frac{-BGAIN}{R.T}}dt\right)^{model}$$

$$e_{Zro2}(t+dt) = \left(\left(e_{Zro2}(t)\right)^{\frac{1}{model}} + ATHIC.e^{\frac{-BTHIC}{R.T}}dt\right)^{model}$$

```
…..
STRUCTURE MODEL NAME 'BEST-FIT' LAW 'COEFF' VARIABLE 'T' VUNIT 'K' RUNLOW 0. RUNUPP 5000.
  SRG VALUE AGAIN 384.944D0 BGAIN 2.47586D5 ATHIC 1.4213D-5 BTHIC 2.47586D5 MODEL 0.5 TERM
  X  1798.K
  SRG VALUE AGAIN 384.944D0 BGAIN 2.47586D5 ATHIC 1.4213D-5 BTHIC 2.47586D5 MODEL 0.5 TERM
  X  1900.K
  SRG VALUE AGAIN 384.944D0 BGAIN 2.47586D5 ATHIC 1.4213D-5 BTHIC 2.47586D5 MODEL 0.5 TERM
 END
```

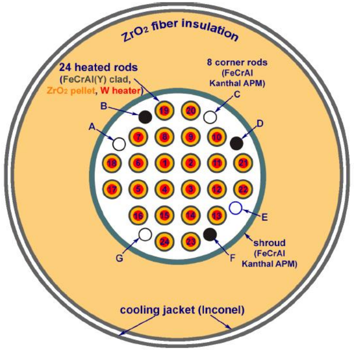
Gabrielli, F., Sanchez-Espinoza, V.H., Wang, S. 2020. ASTEC modelling capabilities for analyzing the QUENCH-ATF tests, Experts' Meeting for the NEA joint undertaking QUENCH-ATF, OECD/NEA, Paris.

Summary of the Current FeCrAl Modeling



Code	Oxidation of	Enthalpy (J/kg)
AC2/ATHLET-CD	Al	$-9.36 \cdot 10^6$
ASTEC	Zr	$-8.93 \cdot 10^6$
MELCOR	Fe (74 wt.%)	$-2.495 \cdot 10^5$
	Cr (21 wt.%)	$-2.442 \cdot 10^6$
	Al (5 wt.%)	$-1.51 \cdot 10^7$

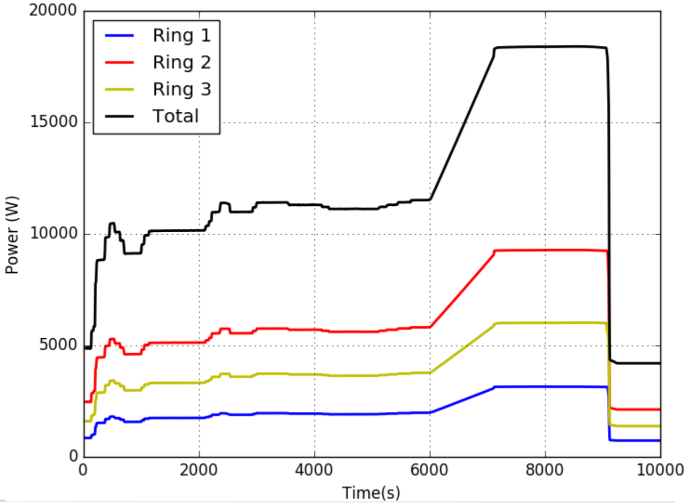
QUENCH-19 Test



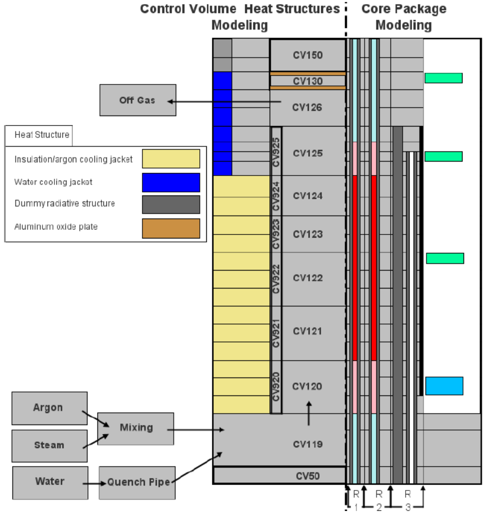
- Heated rods grouped in three radial rings:
  - Inner: 4 rods
  - Middle: 12 rods
  - Outer: 8 rods

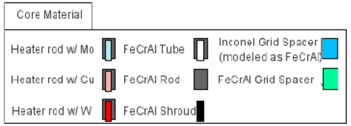
- Phase 1: heating up to ~600 °C (4 kW).
- Phase 2: power increase up to 11.5 kW (pre-oxidation).
- Phase 3: power increased up to 18.12 kW (5 W/s) (T_{pct}~1500 °C).
- Phase 4: power reduced to 4.1 kW.

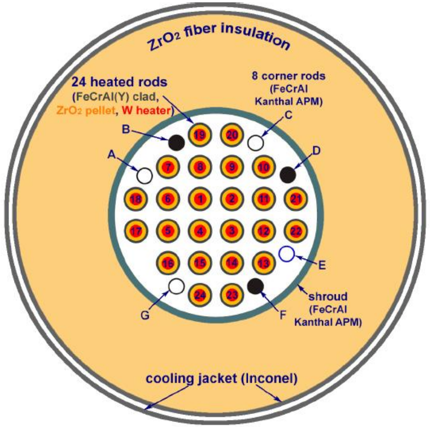
- Atmosphere of Ar (3.45 g/s) and superheated steam (3.6 g/s).
- Reflooding at ~9100 s
  - Fast initial injection of 4 kg of water
  - Slow injection 48 ~ g/s of water

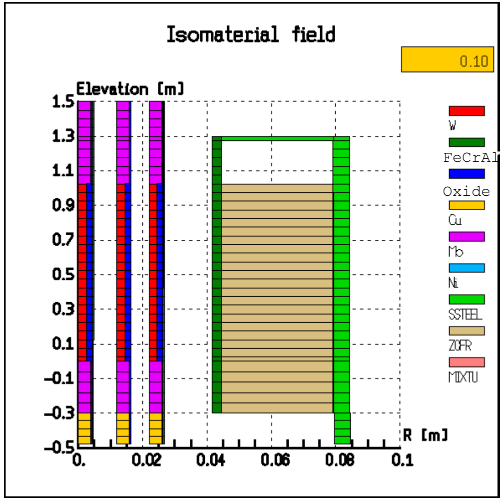


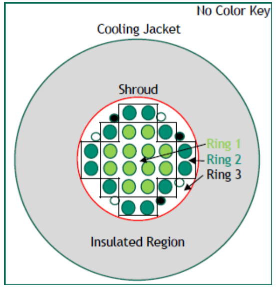
QUENCH-19 MELCOR and ASTEC Models

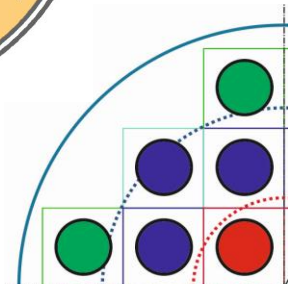










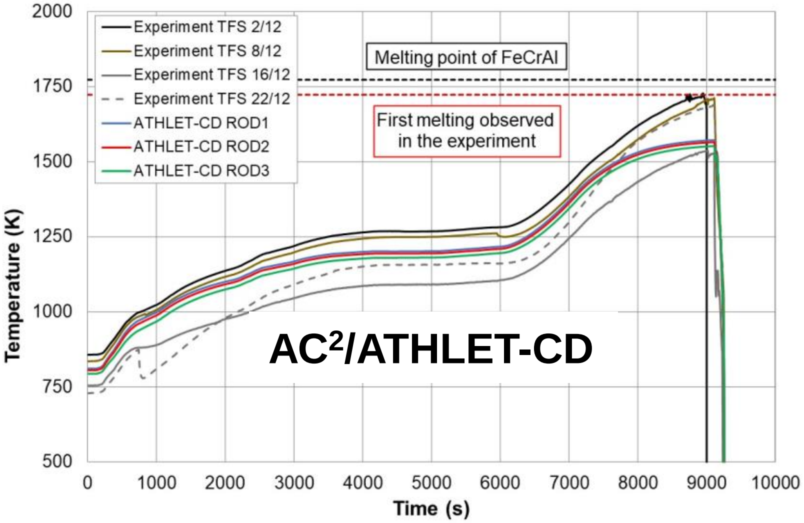


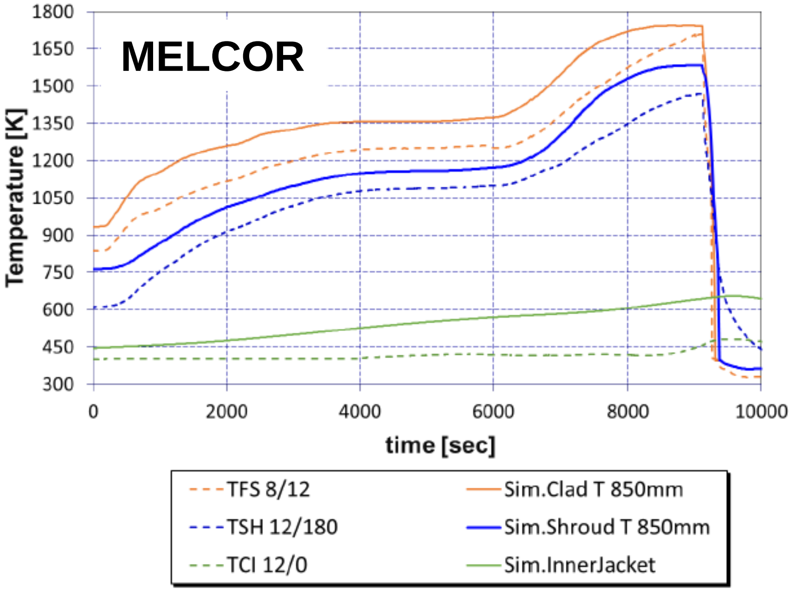
Ch. 3, 8 rods, r_{ext}= 41.5 cm

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

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

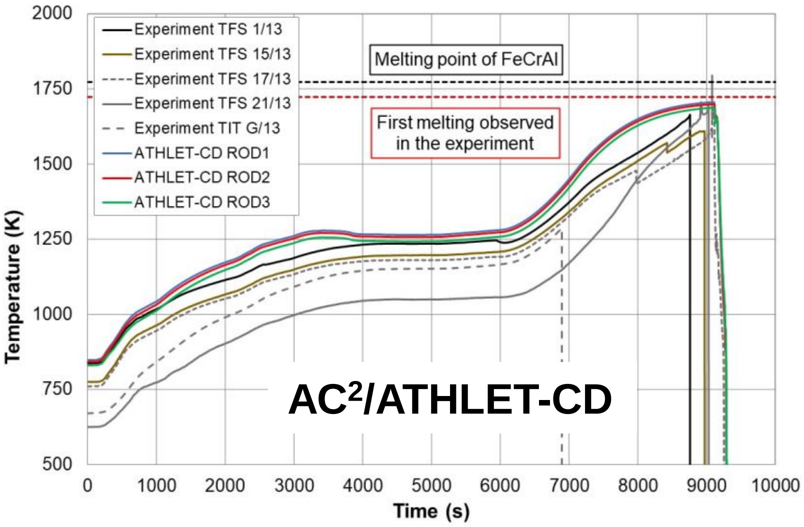
Preliminary results: Clad Temp. @850 mm Height

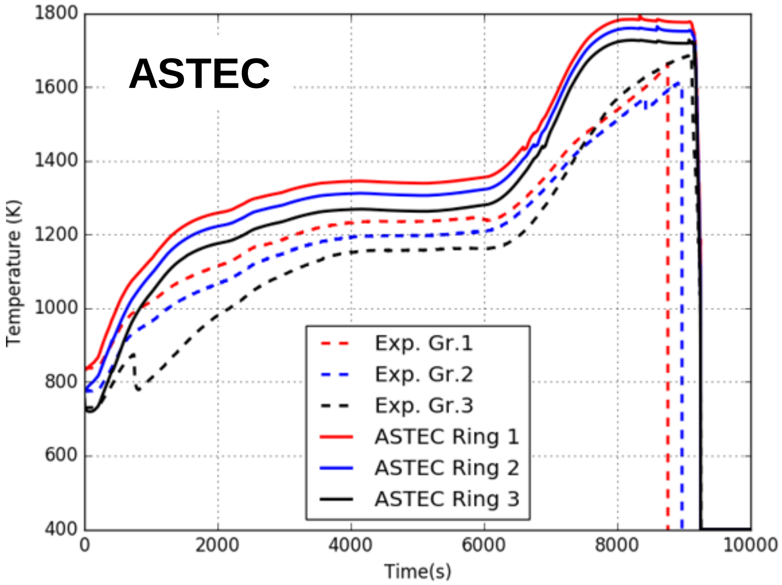




- Simulation of clad temperatures presently exceeds the experimental data.
- No temperature escalation is calculated as shown in the test.

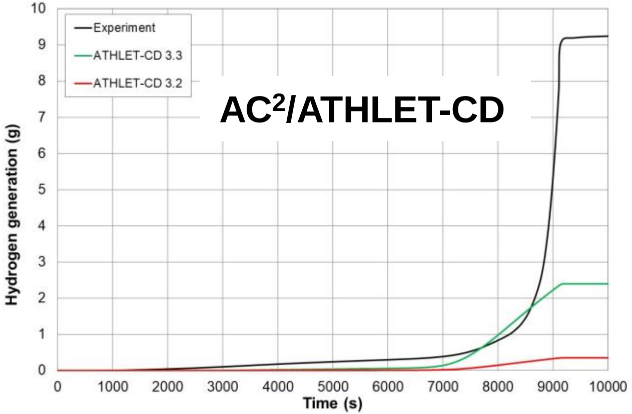
Preliminary results: Clad Temp. @950 mm Height

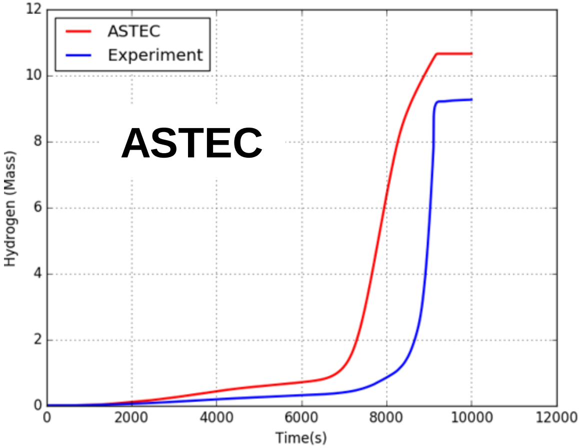


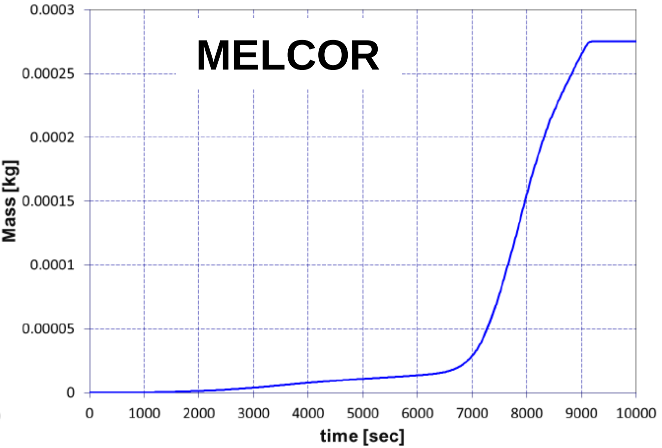


- ➢ No further temperature increase during quenching in agreement with the test.
- ➢ Good agreement of temperatures within heated length, but overestimation of temperatures above heated length observed.

Preliminary results: Hydrogen Production







- MELCOR (0.27 g) predict a much lower H_2 production than the experiment (9 g).
- AC^2/ATHLET-CD (2.4 g) still underpredicts the H_2 production. The new code version shows better results than first approaches.
- ASTEC results look reproducing the time-dependent behavior of the experiment (larger oxidation rate employed in the model).

Conclusions

- Efforts are going on to extend the capabilities of the AC^2/ATHLET-CD, ASTEC, and MELCOR codes to model the ATFs.
- A dedicated FeCrAl material has been implemented in the codes.
- The QUENCH-19 test has been employed for validating the new models.
- Preliminary results of the clad temperatures
  - Simulations exceed the experimental data
  - No escalation as well as no further temperature increase during quenching observed as in the test
- Preliminary results of the H_2 generation
  - MELCOR simulations significantly underestimates the experimental data
  - AC^2/ATHLET-CD simulations still underestimates the experimental data, but improved modelling
  - ASTEC predictions look qualitatively reproducing the experimental behavior
- Modeling and results still evolving.
- QUENCH-19 analysis a solid basis of understanding for further refinement of the models also in view of the activities in the OECD/NEA QUENCH-ATF project and IAEA CRP ATF-TS.