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PSI air oxidation model in MELCOR: Part 2: Analysis of experiments and model assessment

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OUTLINE

- PSI air oxidation model, main assumptions
- Description of QUENCH-10 and QUENCH-16 experiments
- Assesement of PSI air oxidation model with Q-10 and Q-16
  - Pre-oxidation
  - Oxygen consumption
  - Reflood
- Conclusions

PSI "air" oxidation model

- The model has been implemented in a local version of M1.8.6_YV

$$Zr + O_2 \rightarrow ZrO_2 \qquad \Delta H^\circ \quad -1098.3\ \text{kJ/mol(Zr)}$$
$$Zr + 2H_2O \rightarrow ZrO_2 + 2H_2 \qquad \Delta H^\circ \quad -588.4\ \text{kJ/mol(Zr)}$$

- Steam oxidation takes place only in the absence of oxygen

- Nitrogen is not a reactive species but it is consider as a catalyze species.

- Breakaway of the oxide film has a dominant role during air oxidation

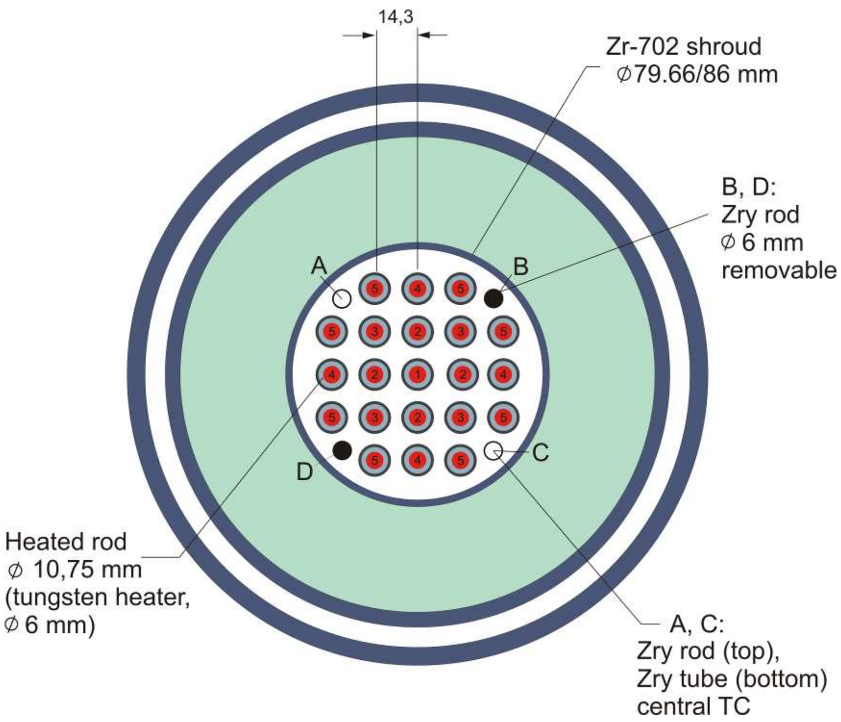
- Breakaway condition is defined as an upper limit on effective oxide thickness

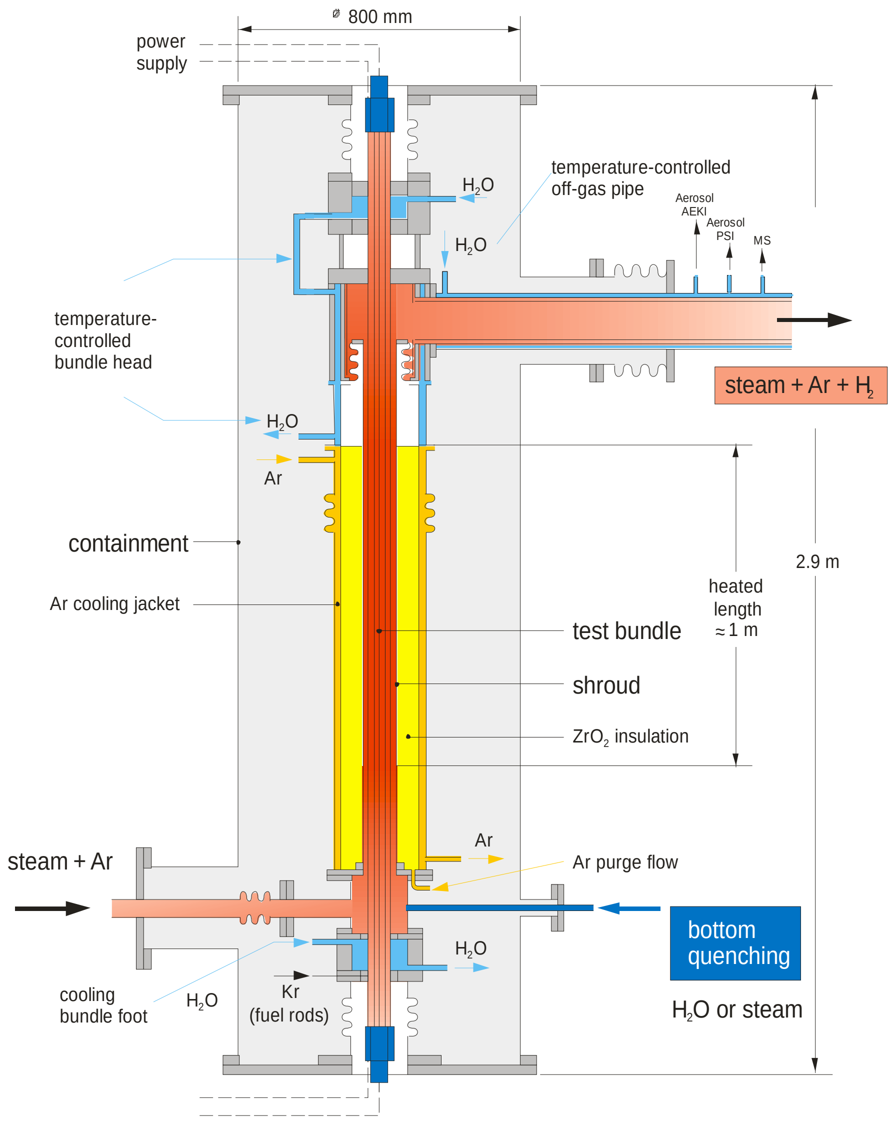
- The steam and air kinetics are very similar without breakaway, when breakaway occurs the kinetics are accelerated.

- Now that the model is successfully implemented in MELCOR we can perform validation studies against integral data.

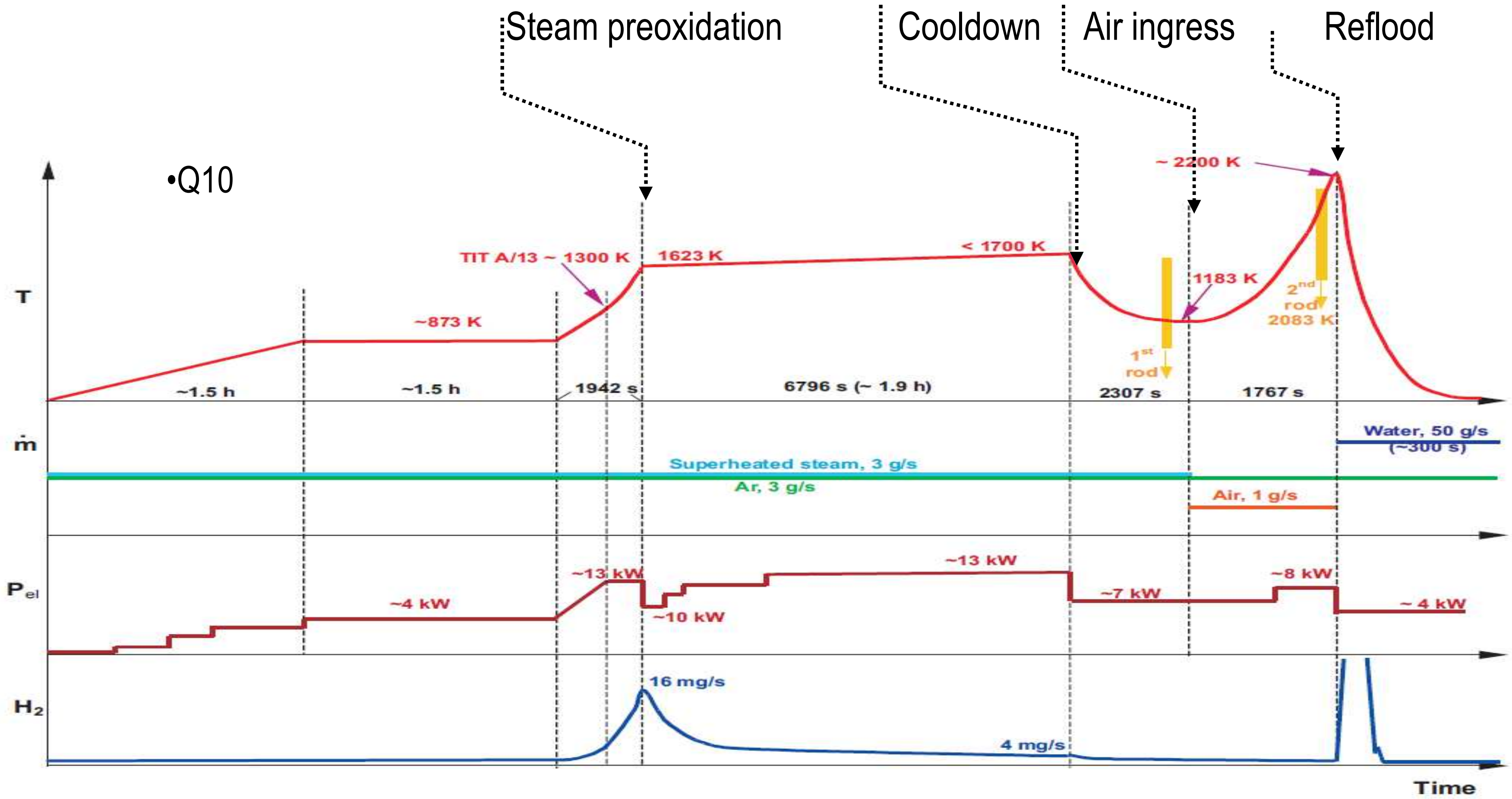
QUENCH Facility

QUENCH facility: electrically heated fuel rod simulator assembly
Operated by Karlsruhe Institute of Technology
ZrO_2 pellets; Zry-4 cladding





QUENCH-10 -16 transient



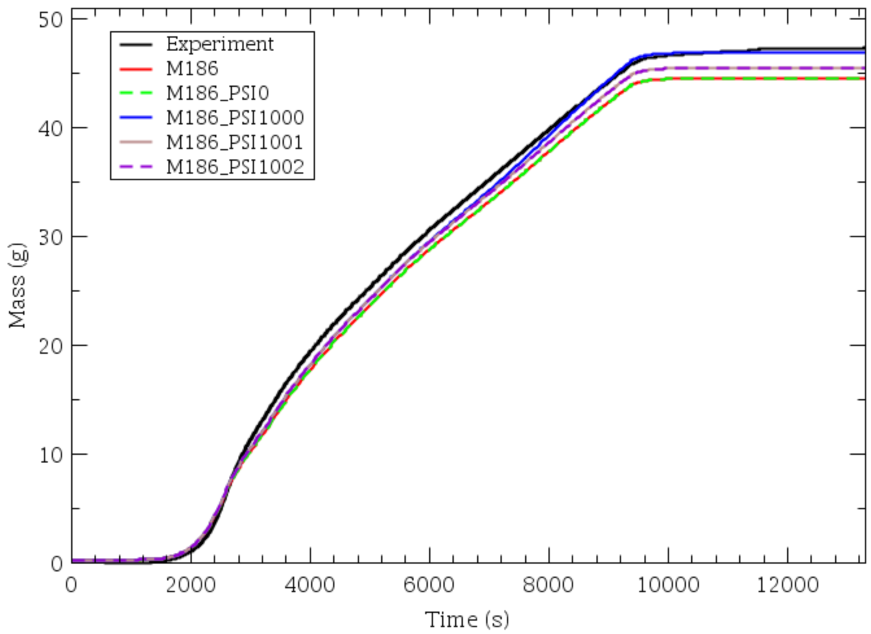
•Q16 was qualitatively very similar but quantitatively different

•Main differences:

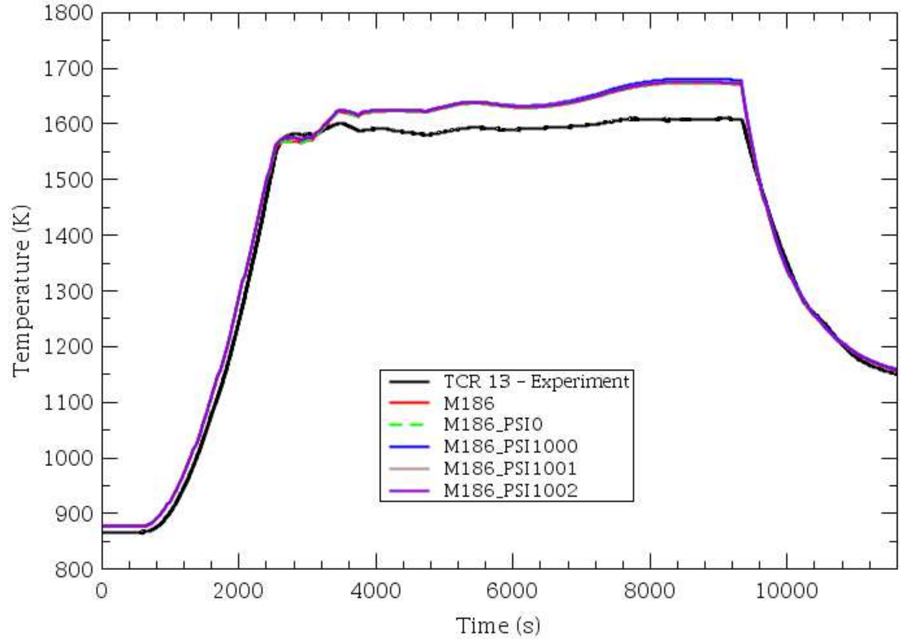
- Lower pre-oxidation (lower T)
- Lower O_2 concentration
- Longer starvation

Q-10 steam phase

Hydrogen generation



Temperature @ 950 mm elevation

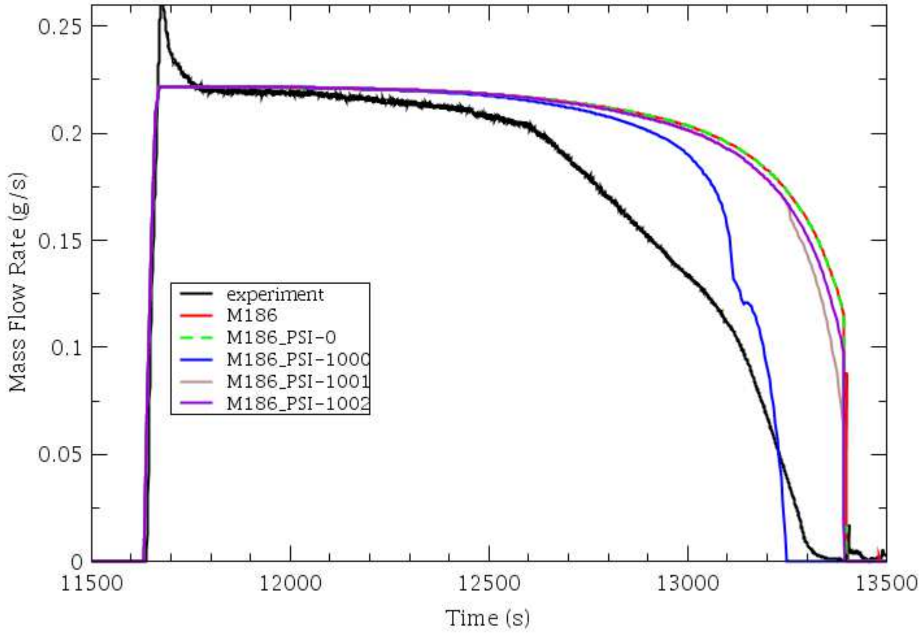


Melcor186	standard MELCOR
M186_PSI0	PSI off (standard MELCOR)
M186_PSI1000	PSI on bkwy steam on and air on
M186_PSI1001	PSI on bkwy steam off and air on
M186_PSI1002	PSI on bkwy steam off and air off

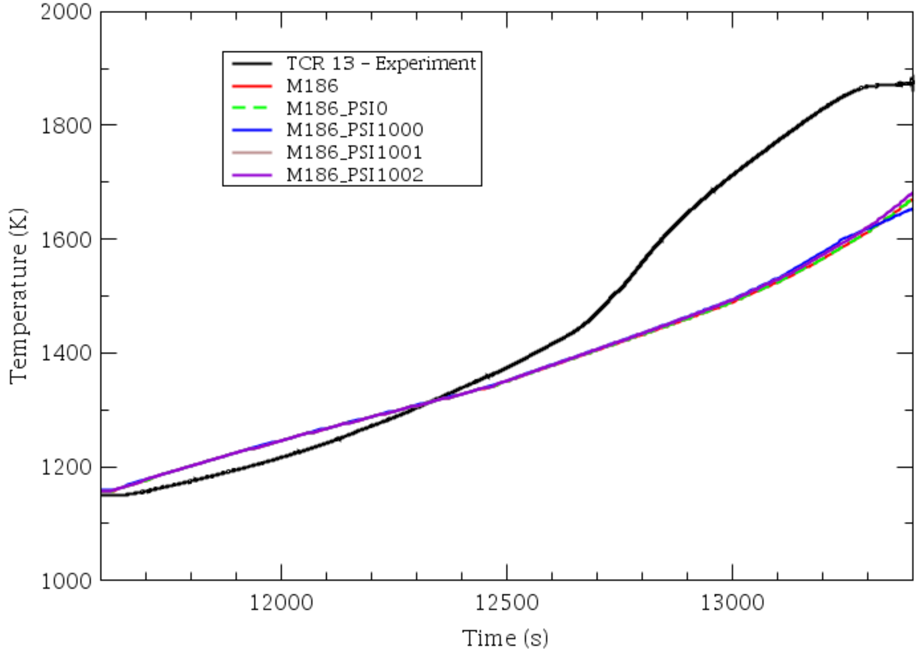
- Maximum temperature and hydrogen generation in fair agreement during the preoxidation phase
- The calculated results with the new code version M186_PSI0 are consistent with Melcor186

Q-10: Air phase

Oxygen mass flow rate at the exit of the bundle



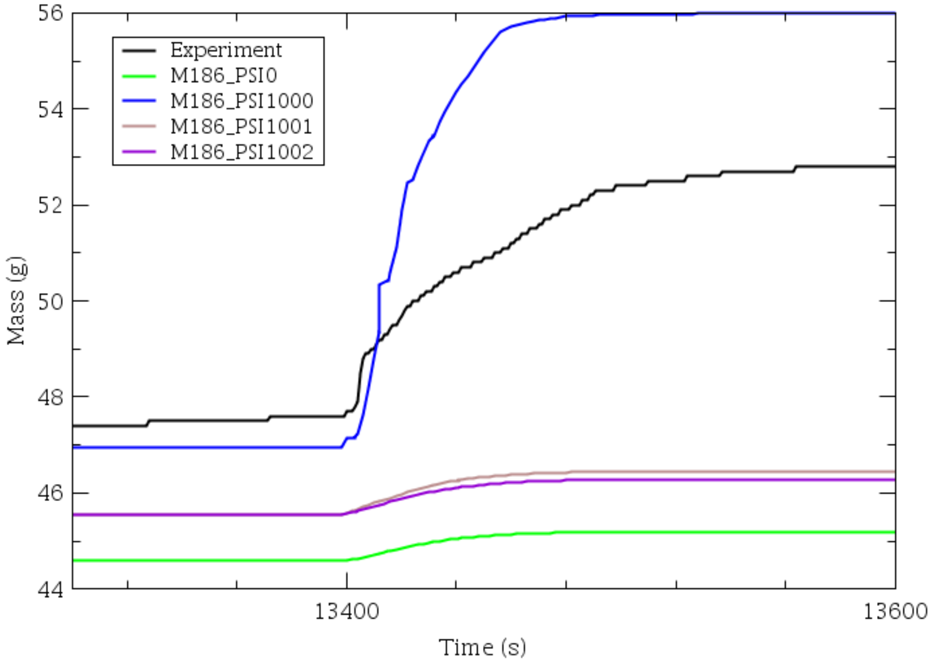
Temperature @ 950 mm elevation



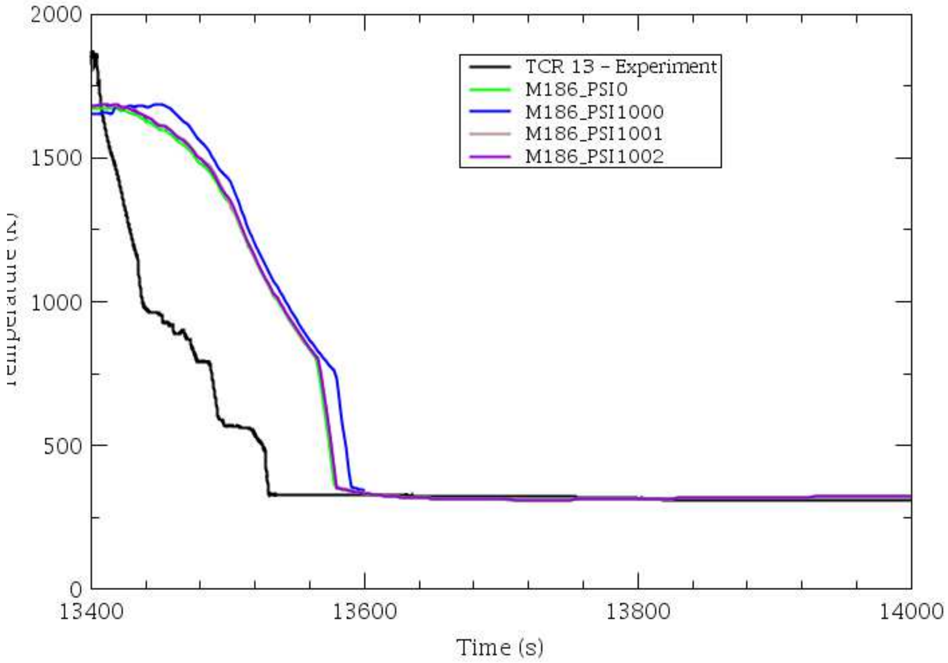
- M186, M186_PSI-0, M186_PSI1001 (bkwy steam off and air on), M186_PSI1001 (bkwy steam off and air off), did not calculate starvation during the air phase.
- M186_PSI1001 did calculate breakaway but later than observed
- Only M186_PSI1000 predicted oxygen starvation and did calculated breakaway

Q10: Reflood

Hydrogen generation



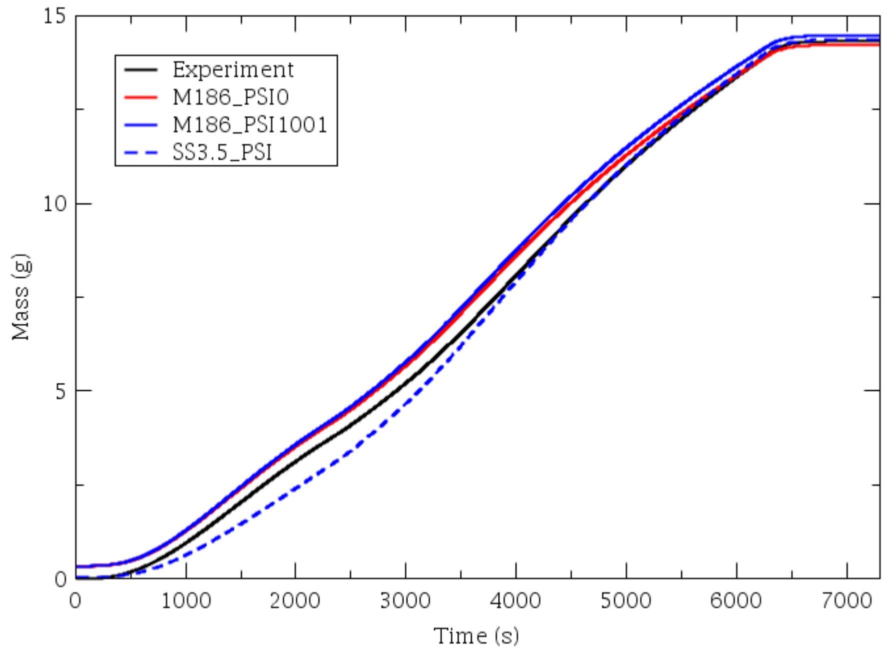
Temperature @ 950 mm elevation



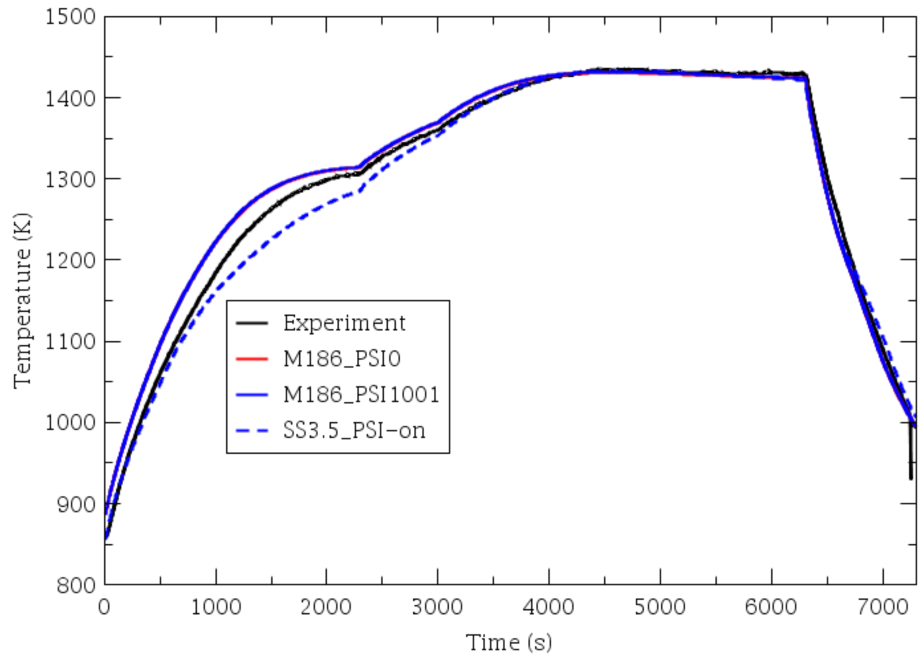
- A very mild excusion and hydrogen generation was observed during reflood
- M186_PSI1000 slightly over predicted it
- M186_PSI-0, M186_PSI1001 (bkwy steam off and air on), M186_PSI1001 (bkwy steam off and air off), slightly under predicted it.

Q-16 Preoxidation with steam

Hydrogen generation

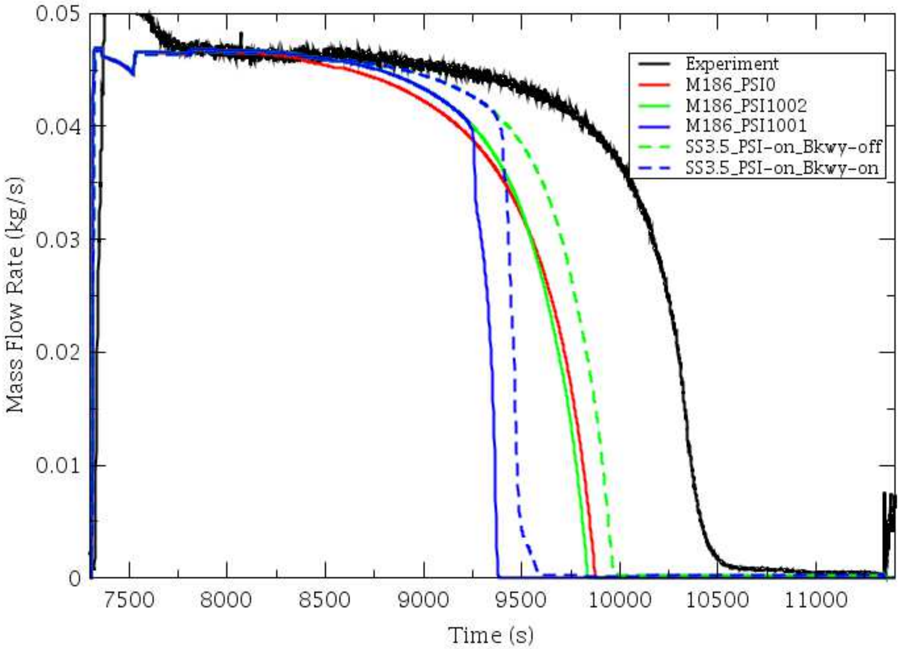


Temperature @ 950 mm elevation



- The calculated temperatues and hydrogen generation are in good agreement with the experimental results
- Similar results are obtained with SCDAP when the same physical models are used

Q16: Air phase / Oxygen consumption

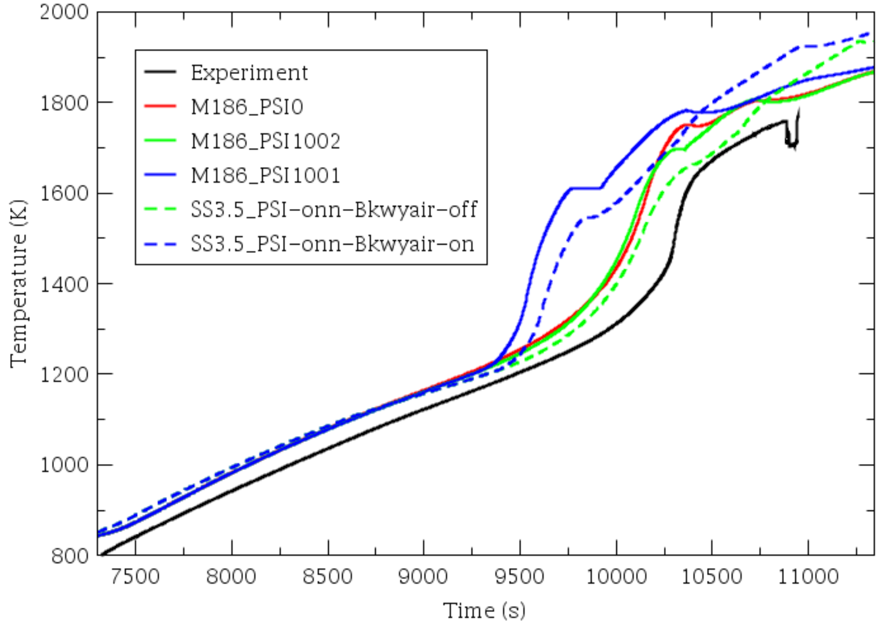


- M186_PSI0 and M186_PSI1002 calculates similar results as expected
  - small difference due to slight diff in oxidation kinetics
- Breakaway was expected during Q16 and it was calculated when breakaway was enabled (M186_PSI1001)

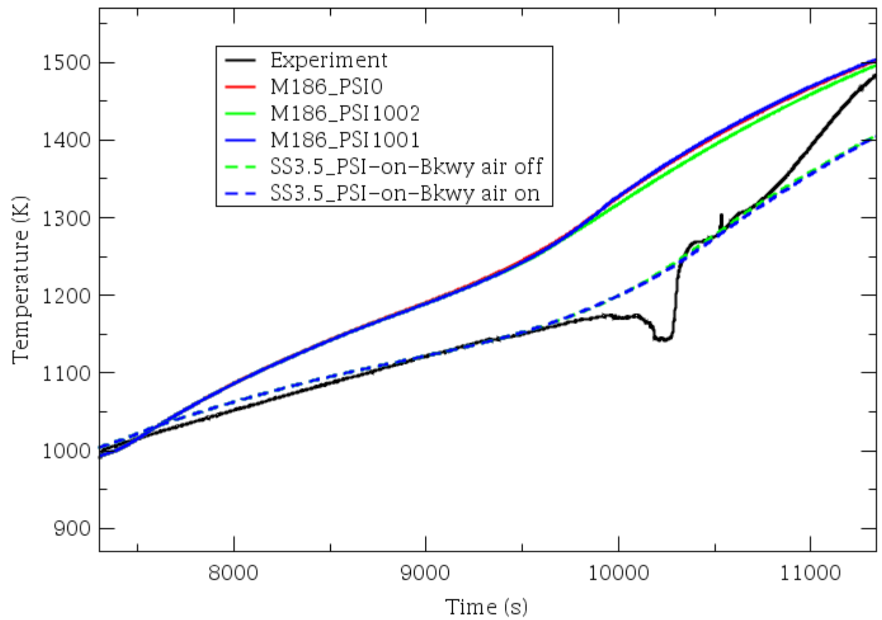
- There was no indication from thermal response or oxygen consumption that breakaway occurred in the experiment.
- This is consistent with the simulation where breakaway was disabled (M186_PSI1002).
- Post-test examinations showed influence of nitrogen at locations which were not oxygen starved.
- All cases predicted earlier oxygen starvation than observed in the experiment even with breakawy disabled.

Q16: air phase

Temperature @ 550 mm elevation

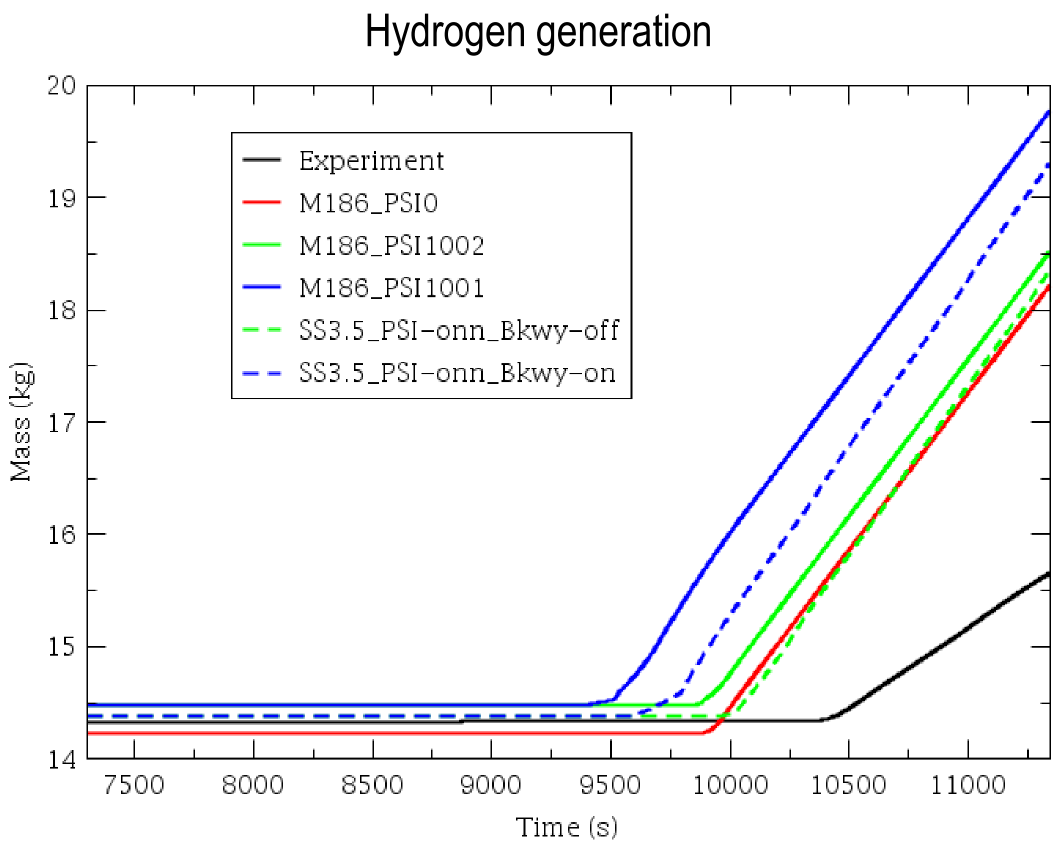


Temperature @ 950 mm elevation



- The temperatures start to increase when the oxygen is starved
- The calculation where breakaway was disabled (**M186_PSI1002**) gave the closest temperature agreement

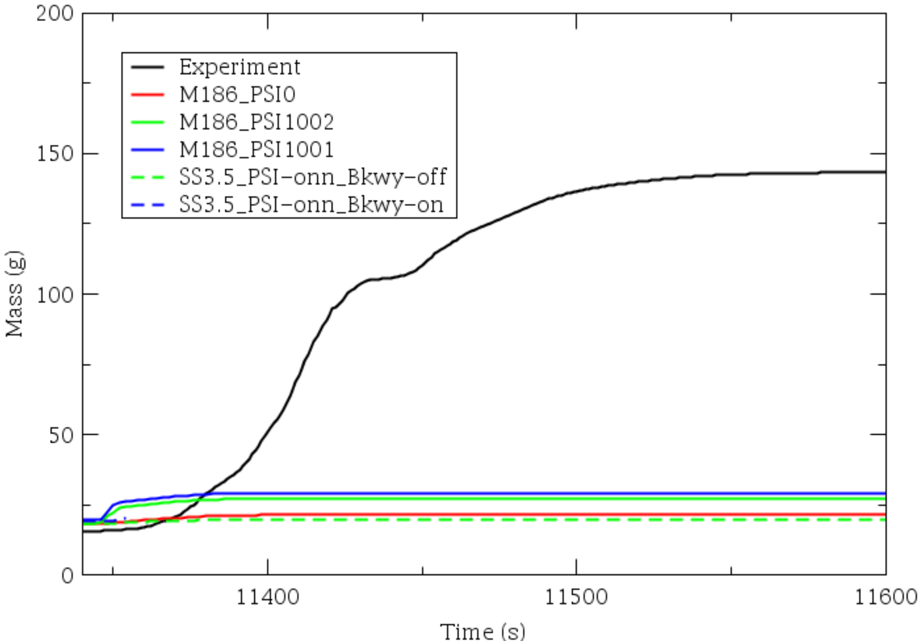
Q-16: H2 generation during the air phase



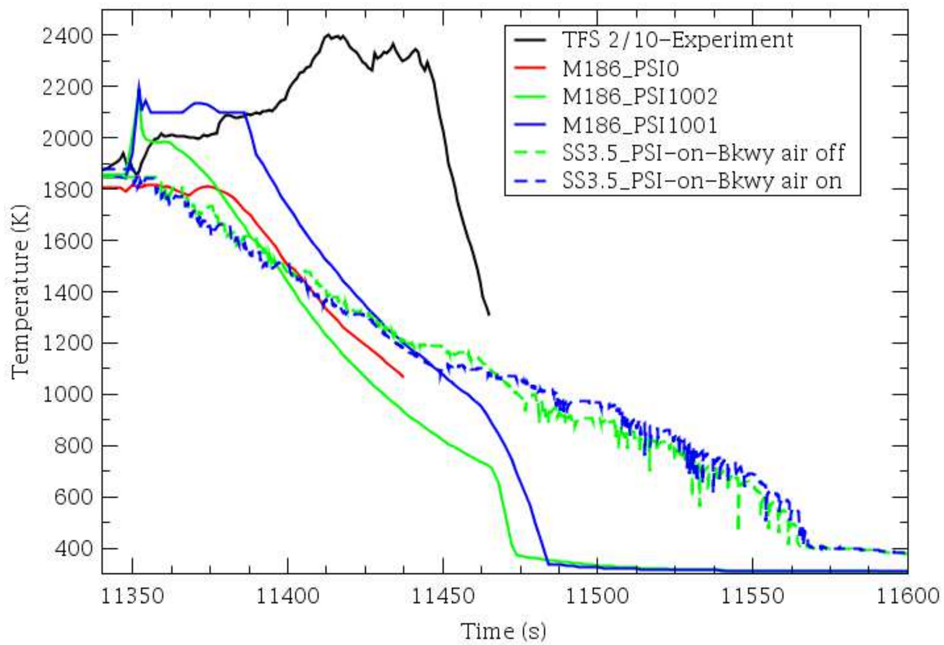
- The model can handle steam and air at the same time
- First the oxygen is consumed and after complete consumption of the oxygen the steam is consumed.

Q16: Reflood

Hydrogen generation



Temperature @ 650 mm elevation



- No excursion was expected for the Q16 experiment
- **High temperatures were observed during reflood**
- Neither of the codes reproduced it:
  - M186_PSI0, SS3.5_PSI_Bkwy-off, and SS3.5_PSI_Bkwy-on predicted no excursion
  - M186_PSI1001 and M186_PSI1002 calculated a mild excursion
- Neither of the codes calculated anywhere near the total **hydrogen production** observed during reflood

Q16: Reflood – possible causes of the excursion

- Possible mechanism for triggering the strong oxidation:

  – **ZrN formation**
    – Experiment showed evidence of nitrogen uptake (about 29g).
    – Nitrides may have weakened the oxide layer
    – the thermo stresses during reflood promoted breakaway
    – Neither MELCOR nor SCDAP are able to predict a nitride reaction

  – **reoxidation of the ZrN and nitrogen release during reflood**
    – evidence of nitrogen release (about **24g**) during the reflood
    – During this time the reaction: $ZrN + 2H_2O = ZrO_2 + 1/2N_2 + 2H_2$ ΔH° -252.8 kJ/mol(Zr) and lasted for about **200s**.
    – This would correspond to **~2.15 kW** of oxidation heat and **~ 7g of H2. N**owhere near to the experimental value.

  – **dissolution of the oxide into an α-Zr(O) region**
    – An oxygen stabilized α-Zr (O) region may have been formed by diffusion of oxygen from the oxide layer into the underlying metallic layer during the long period of oxygen starvation.
    – oxide layer reduced to α-Zr(O) and increased its susceptibility to oxidise and react with nitrogen.
    – Experience on SET has shown that the α-Zr(O) layer reaction with nitrogen plays an important role during oxidation
    – The codes are not able to model the α-layer formation.

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Conclusions

- The PSI breakaway model was successfully implemented in M186 and assessed against the air ingress experiments Q10 & Q16.

- Breakaway and oxygen starvation were calculated in Q10, but later than observed.

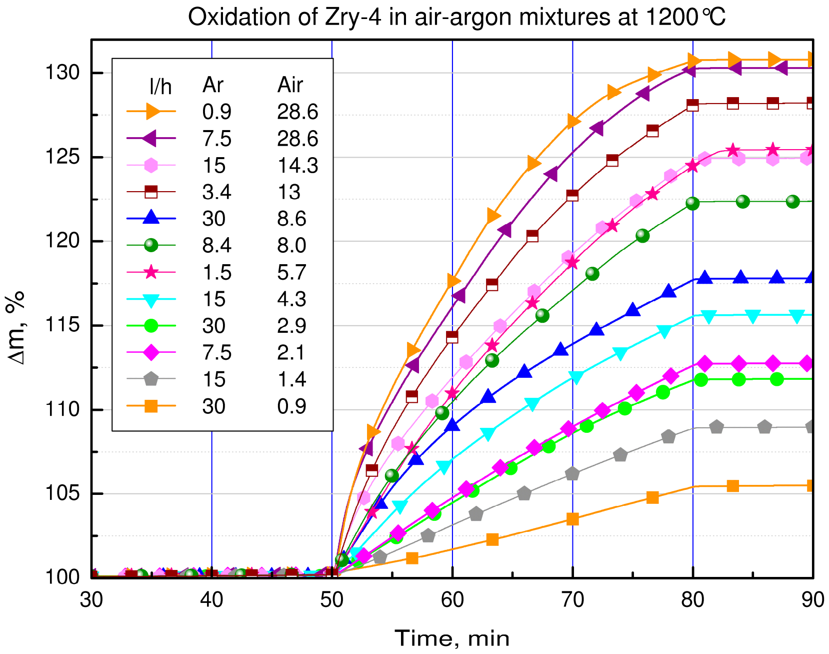
- A mild temperature excursion was observed during the Q10 experiment.
  - Only the calculation with breakaway enable for both steam and air calculated the excursion.

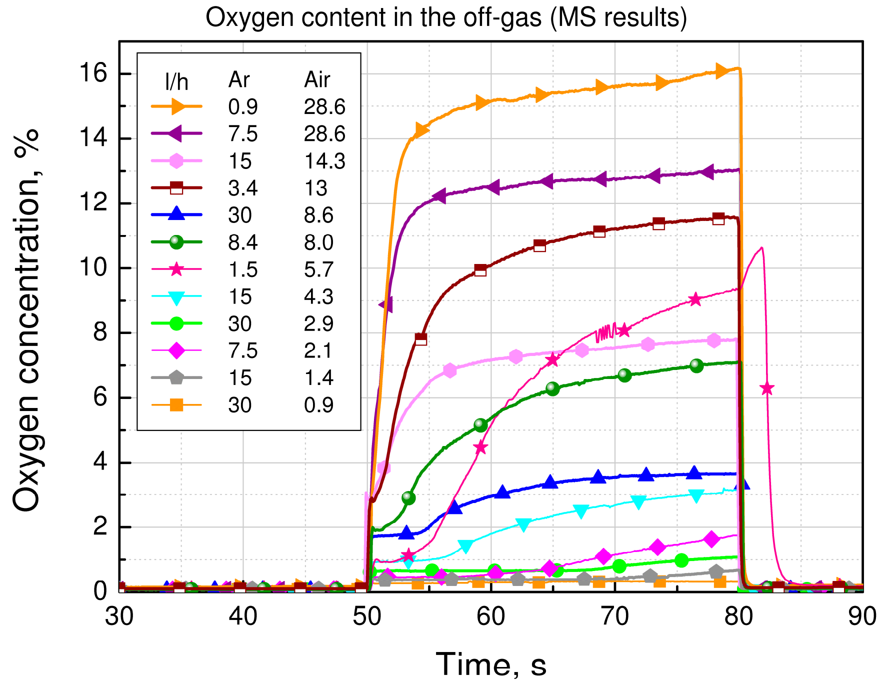
- Breakaway was expected during Q16 and it was calculated when breakaway was enabled.
  - However there was no indication from online measurement that it occurred,
  - and this was supported by the simulation where breakaway was disabled
  - Possible that the low oxygen concentration may have influenced the kinetics and masked the effect of breakaway.
  - Evidence that this may be significant.

- The large excursion observed during reflood in the Q16 experiment was not reproduced.
  - A previously damaged oxide layer,
  - nitride reaction and α-Zr(O) formation
  - or a combination of all may be the cause of the excursion.
  - These are identified as areas where model improvement is necessary

Thank you for your attention

Effect of oxygen concentration on kinetics: data

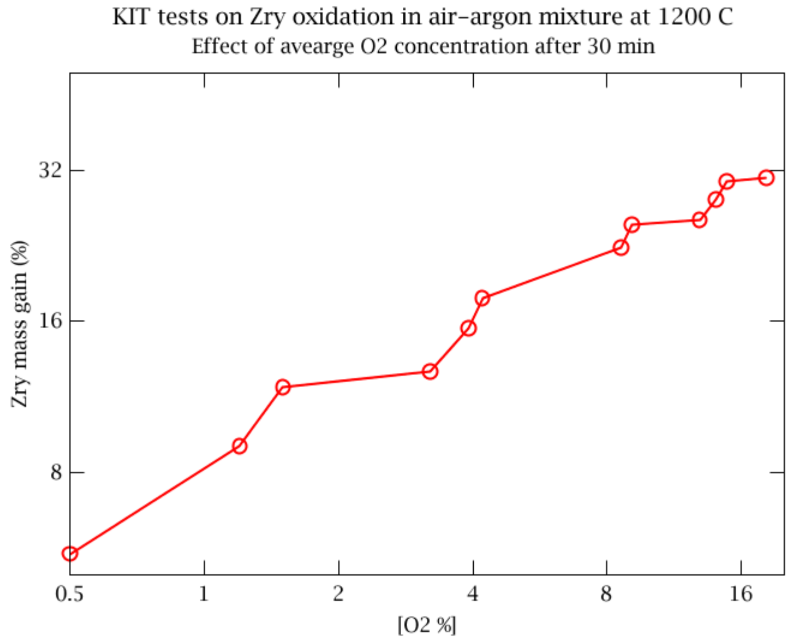


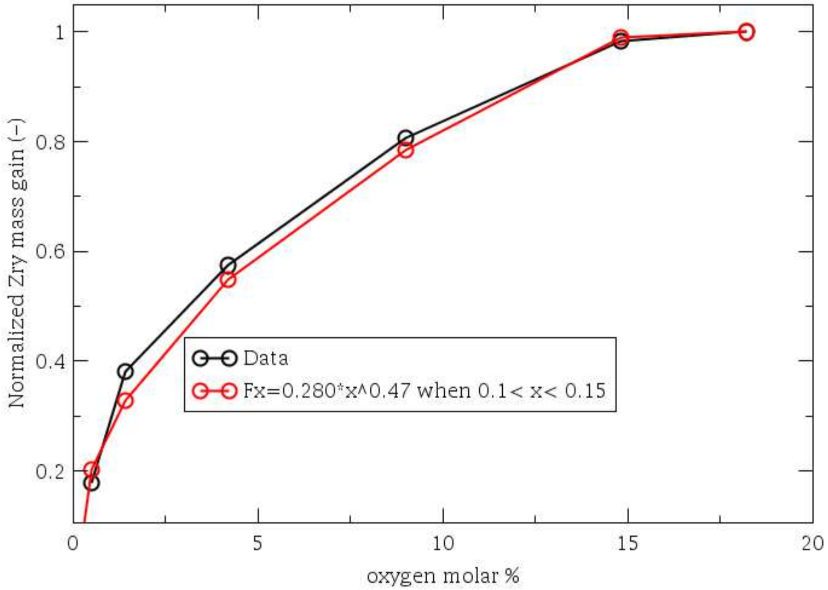


SET‘s from KIT presented during the QWS 17th

The oxidation kinetics depends on oxygen concentration.

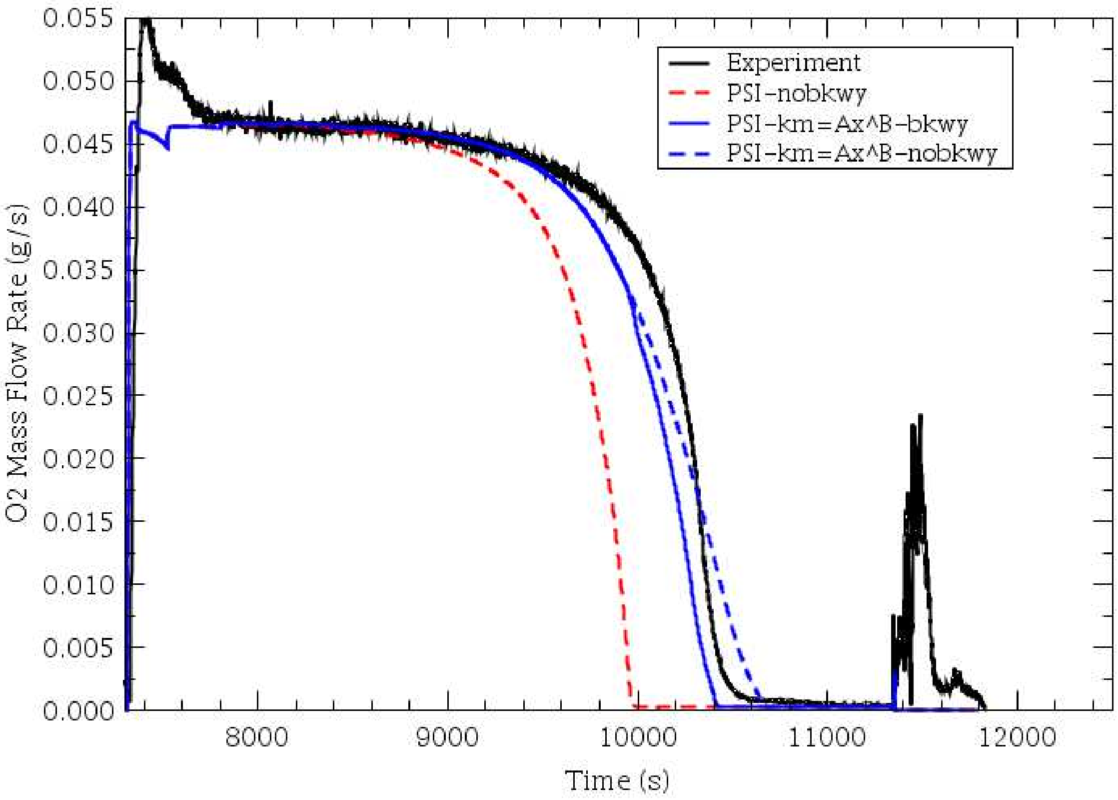
Effect of oxygen concentration on kinetics: correlation





- ➢Time-averaged oxidation was extracted from the results and plotted as a function of mean bundle concentration.
- ➢A curve of dependence was deduced that intended to capture the effect well enough to go into a model.
- ➢Note that this is purely a fit to a limited set data, used to explore the effect. It is not a proposed model

Analysis of Q-16 with SCDAPSim 3.5 with trial correlation



•Red: PSI air oxidation model with/without breakawy

• Blue: including also the correlation for [O2] concentration

•The calculation with breakaway and [O2] concentration are closest to experiment

•If bkwy had occured in the experiment would not have been obvious.