

Project Proposal

Thermal Hydraulics of U-Zr-O molten pool under oxidising conditions in multi-scale approach (crucible - bundle - reactor scales)

Short title: **THOMAS**

(Thermal Hydraulics of Oxidising Melt in Severe (\leftrightarrow) Accidents)

Presented by
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11th Meeting CEG-CM
Forschungszentrum Dresden-Rossendorf (FZD)
March 7-9, 2007

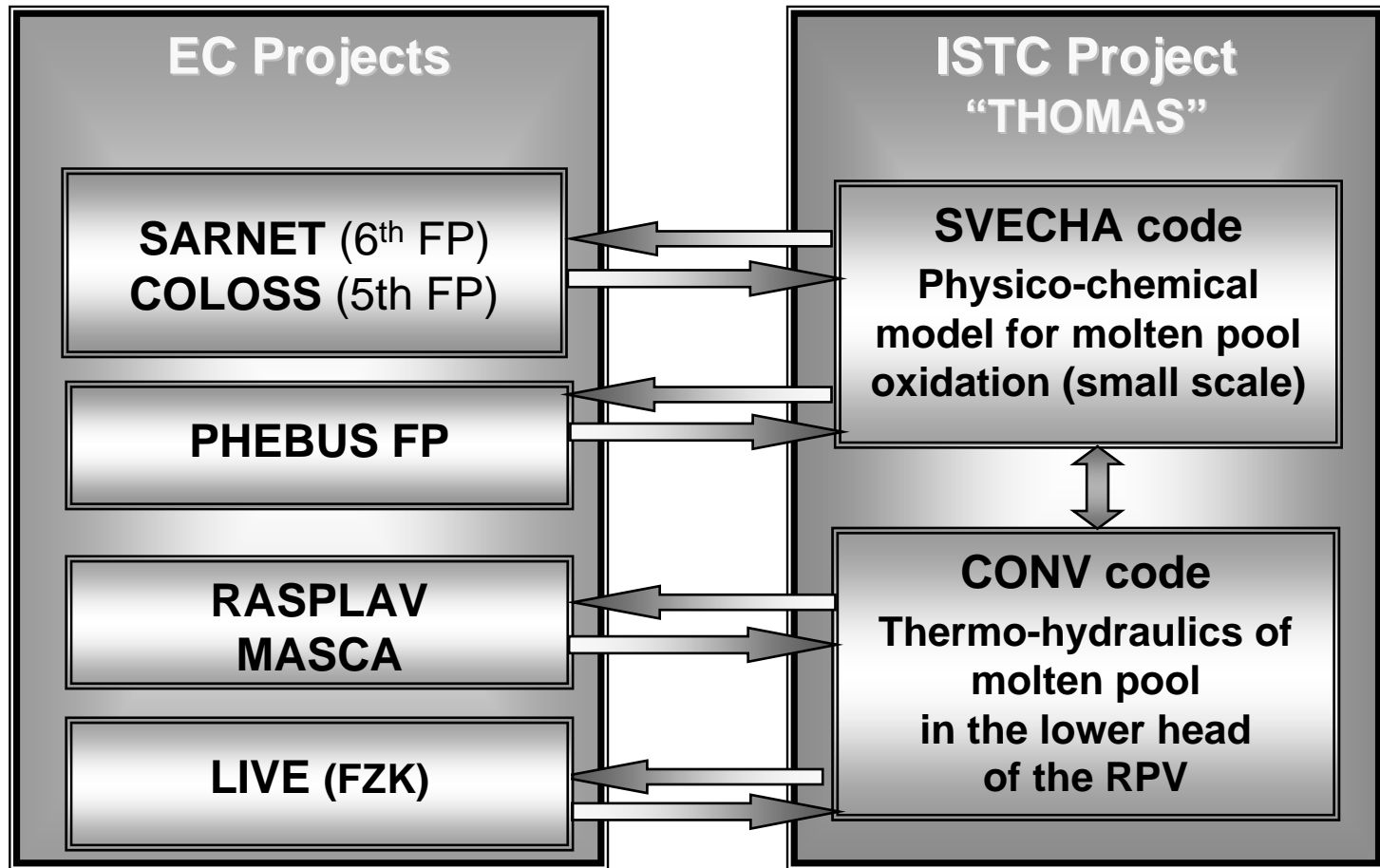
General Information

Leading Institution:	IBRAE, Moscow (Nuclear Safety Institute of Russian Academy of Sciences)
Duration: Commencement:	3 years
Total cost:	\$ 200 000

Project Objectives

- On the base of analysis of available test data from small - and large - scale experiments, to develop a mechanistic description of U-Zr-O molten pool behaviour in oxidising conditions.
- For this purpose, to carry out a tight coupling of the two advanced numerical tools developed within the previous Project #2936: the SVECHA physico-chemical (molten pool oxidation) model and the 3D thermo-hydraulic code CONV.
- This will allow extension of thermal hydraulic consideration of oxidised melt from small scales (crucible tests) up to a large scale (reactor pressure vessel), including an intermediate scale corresponding to molten pools in the bundle tests.
- As a result, improved interpretation of Phebus FP tests observations of corium melt oxidation, as well as transposition of thermal hydraulic consideration from test (e.g. MASCA or RASPLAV) to reactor scale, are foreseen.

Interconnection of the Project with the other Projects



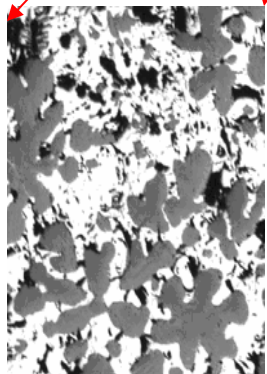
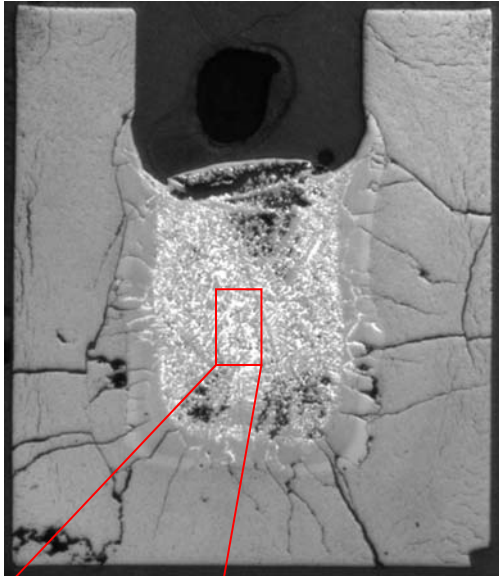
Experimental observations

- Non-destructive and destructive post-test examinations of bundles in various tests showed formation of molten pools of different scales at various stages of core degradation:
 - small local pools in CORA and QUENCH test bundles.
 - extended molten pool in a central zone of the Phebus FP test bundles (similar to TMI-2).
- In the late stage of a severe accident, melt relocates into the lower head of the reactor pressure vessel and forms a large molten pool.
- Oxidation kinetics of melts can be significantly higher in comparison with that of solid materials, therefore, it strongly determines heat and hydrogen source terms during severe accidents (QUENCH tests). On the other hand, the oxidation kinetics strongly depends on thermal hydraulic behaviour of oxidised melt.
- Therefore, investigation of in-vessel molten pool behaviour under oxidation conditions is of paramount importance with respect to core degradation and reactor pressure vessel failure analysis.

Zr melt oxidation in ZrO_2 crucible tests (1/2)

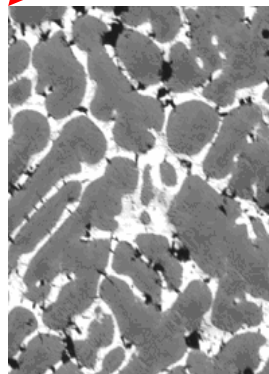
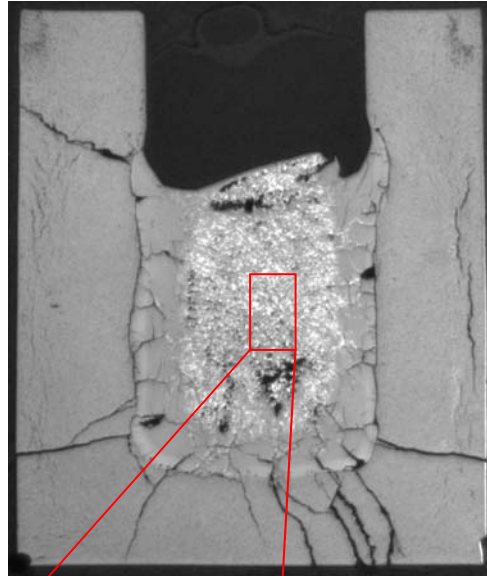
(FZK, J.Stuckert)

T=2200°C



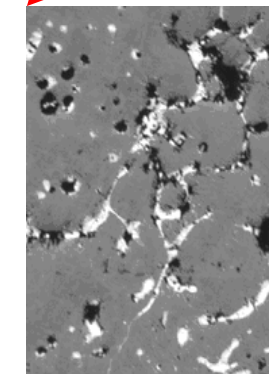
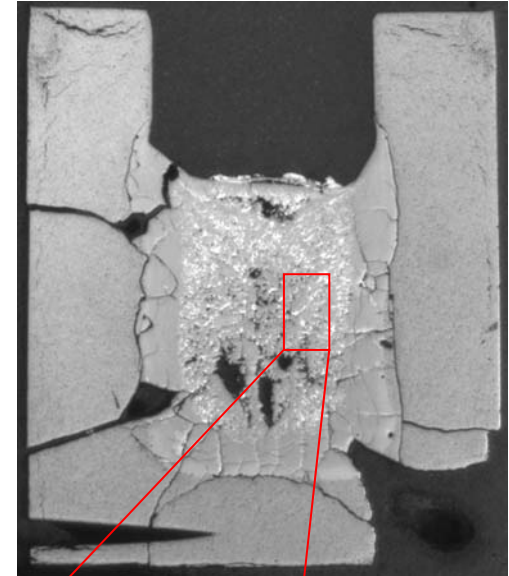
$t = 10$ min.

Zr:O= 42:58



$t = 15$ min.

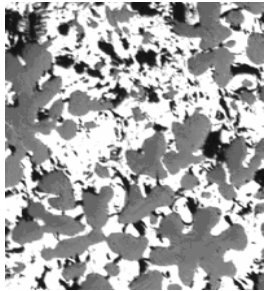
Zr:O= 39:61



$t = 25$ min.

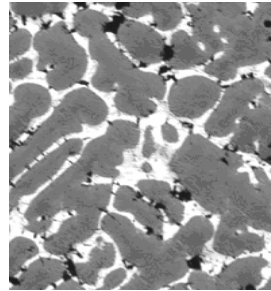
Zr:O= 37:63

Zr melt oxidation in ZrO₂ crucible tests (2/2)



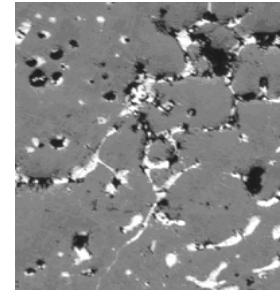
t=10 min.

Zr:O= 42:58



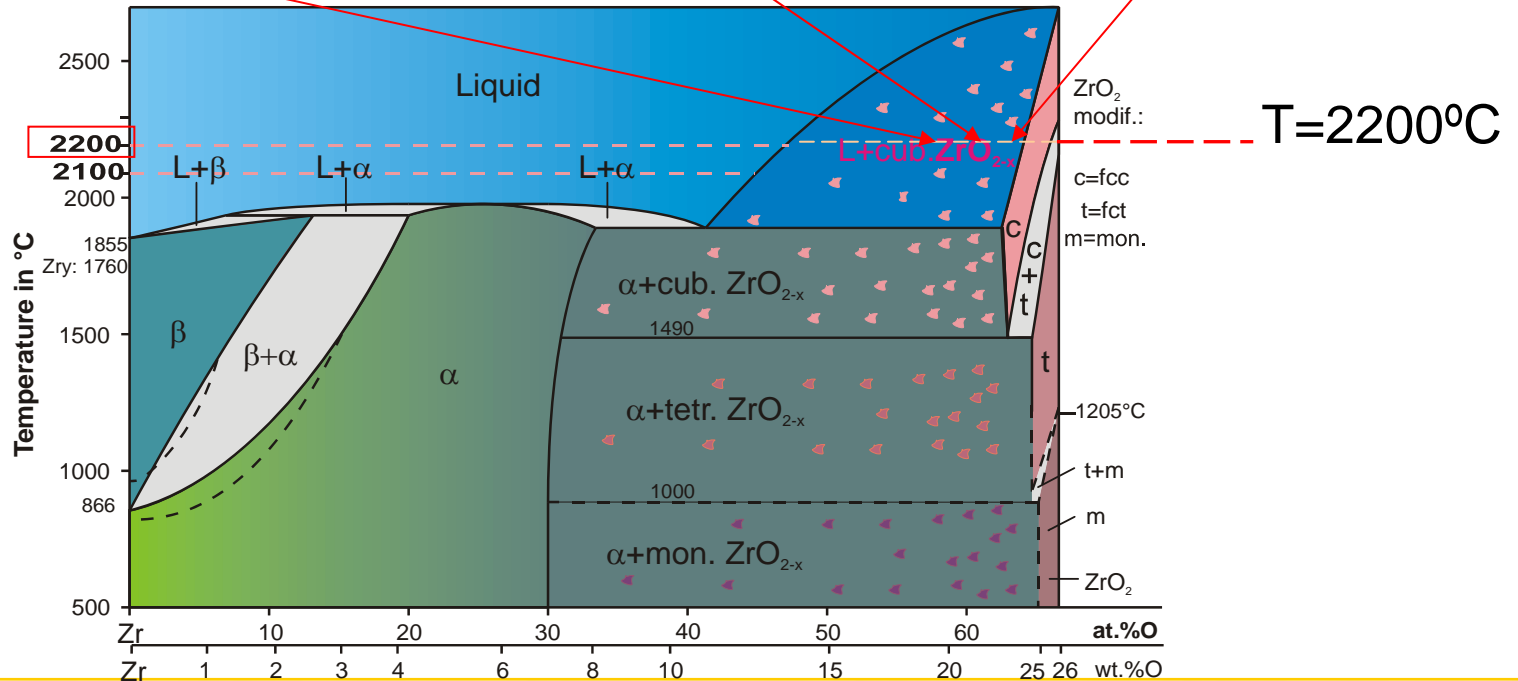
t=15 min.

Zr:O= 39:61



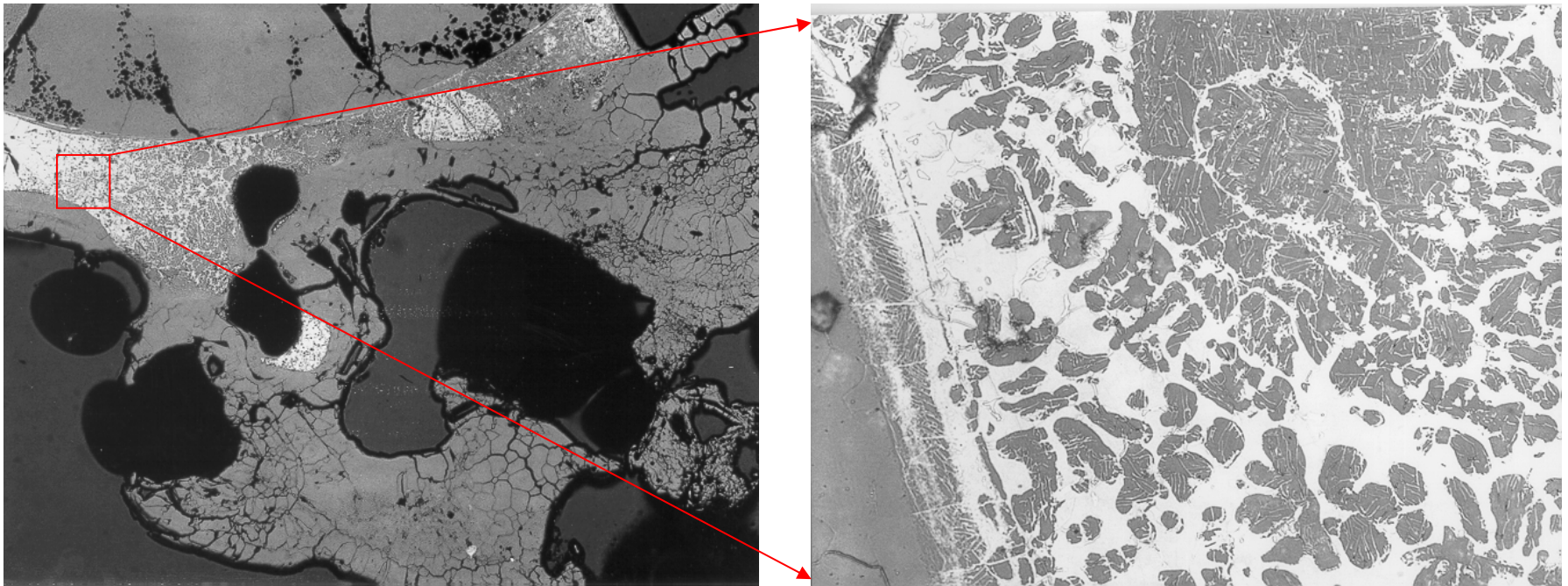
t=25 min.

Zr:O= 37:63



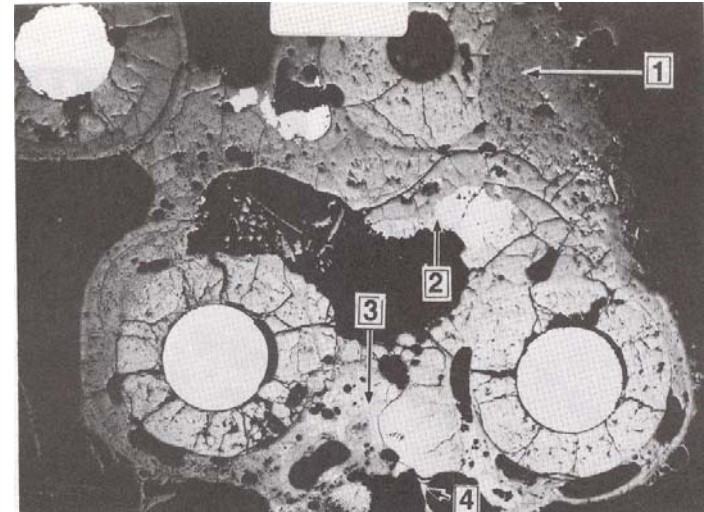
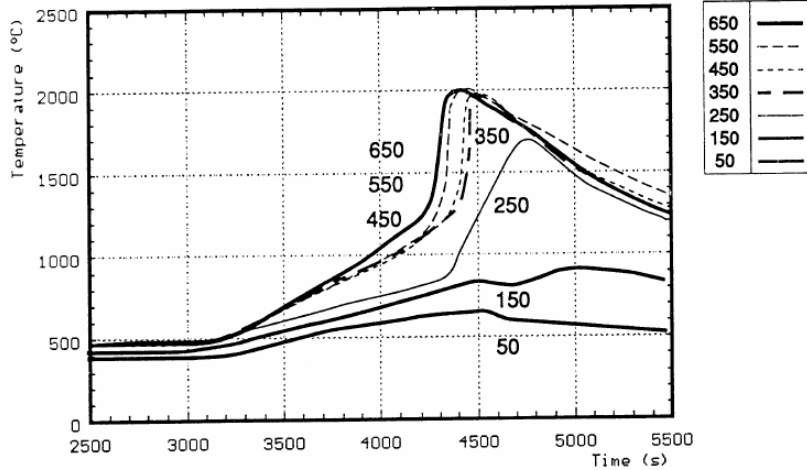
Zr-O melt oxidation in QUENCH tests

Maximum temperature ≈ 2500 K



Cross-section Q-03-05 of QUENCH-03 test bundle at elevation 750 mm.
 “Bulk” oxidation of melt.

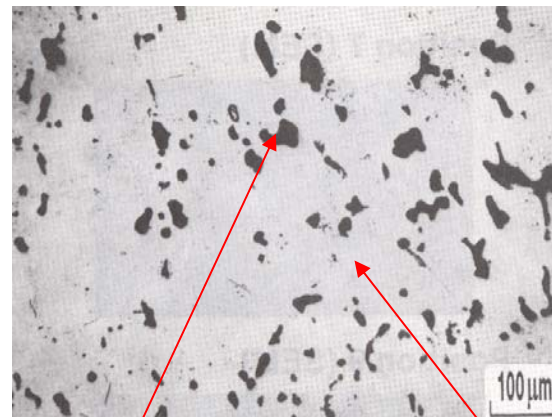
U-Zr-O melt oxidation in CORA tests



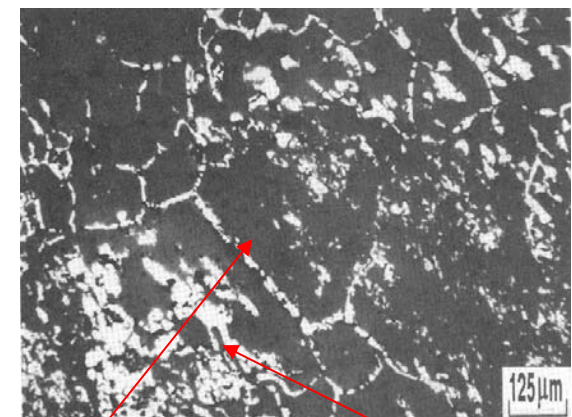
Position 1

Position 3

“Bulk” oxidation of melt.
Best estimate maximum temperature $\approx 2000^\circ\text{C}$



Voids

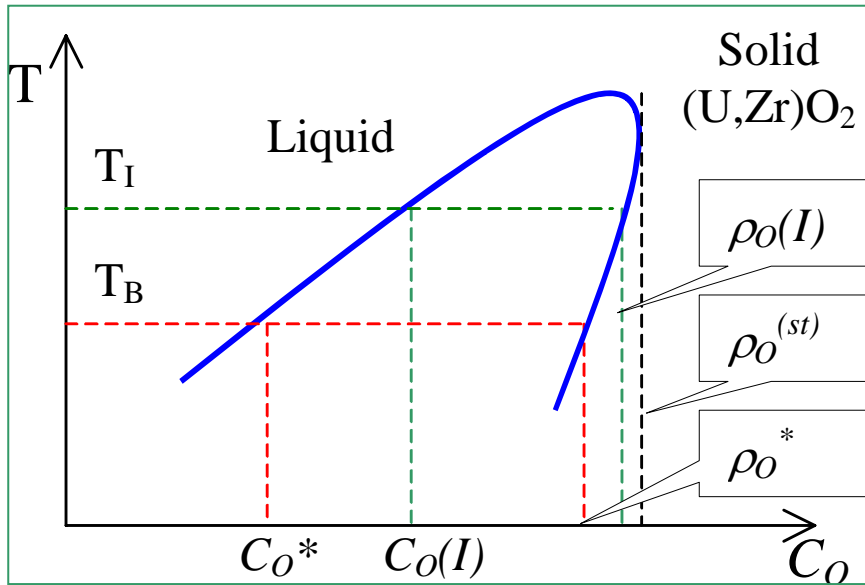
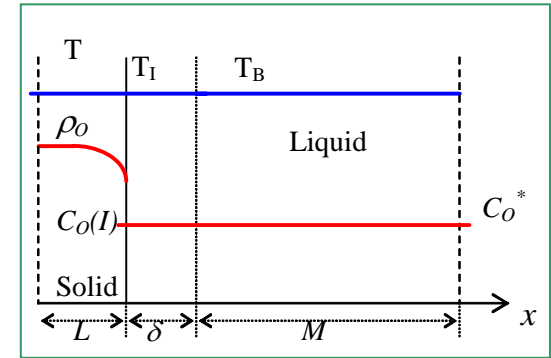


Ceramic phase
(U,Zr)O_{2±x}

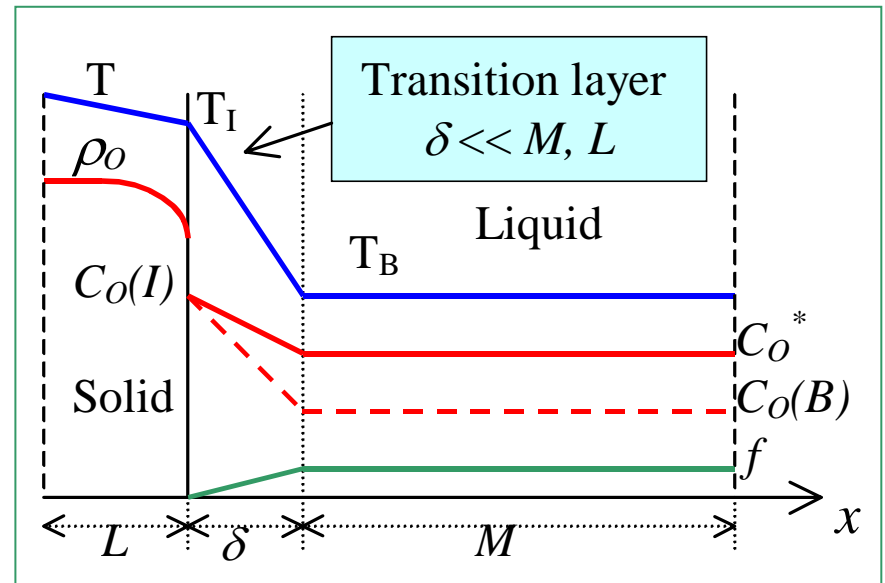
Metal phase
(U,Zr,O)

SVECHA model of U-Zr-O melt non-equilibrium oxidation in steam (1/2)

Melt saturation under isothermal conditions



Fragment of quasi-binary phase diagram



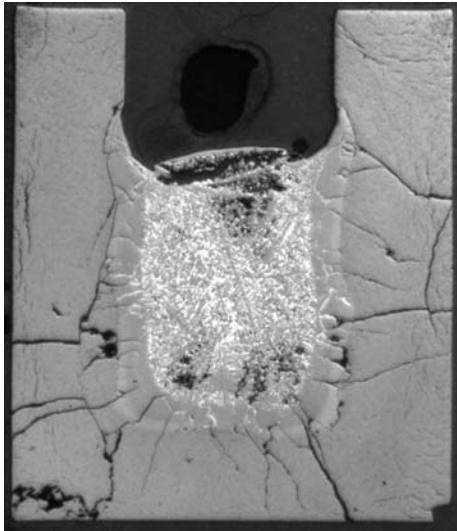
Spatial distribution of temperature and oxygen concentration

SVECHA model of U-Zr-O melt non-equilibrium oxidation in steam (2/2)

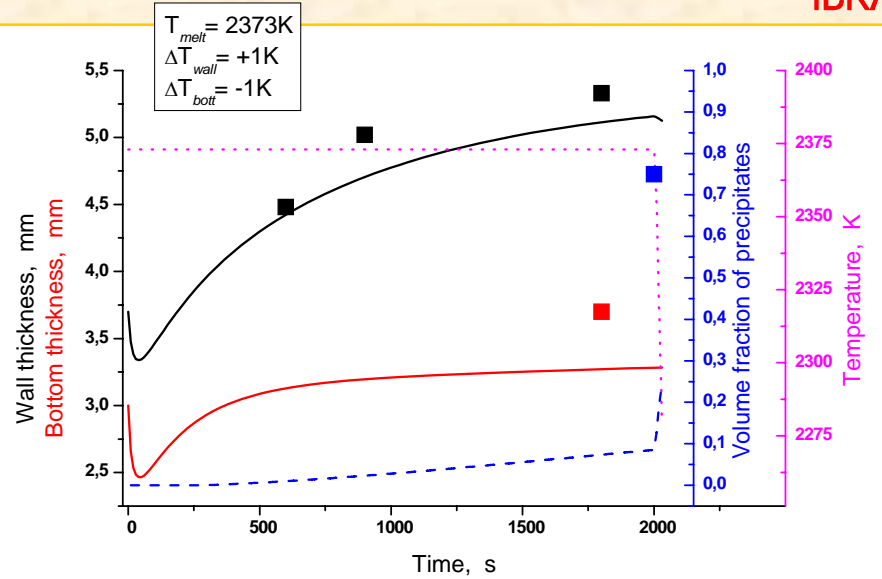
Main findings:

- Melt oxidation as well as UO_2 dissolution under non-equilibrium conditions characterised by temperature difference between solid and liquid phases, can proceed after attainment of the melt saturation and result in the ceramic phase precipitation in the melt bulk (up to complete conversion into ceramic phase).
- Depending on test conditions, the precipitation process can be accompanied with the peripheral oxide layer (crust) growth or dissolution.
- The new model predicts secondary dissolution of oxide crust at a very late stage of interactions. This prediction was confirmed by FZK crucible tests (J.Stuckert), specially designed for comparison with model predictions

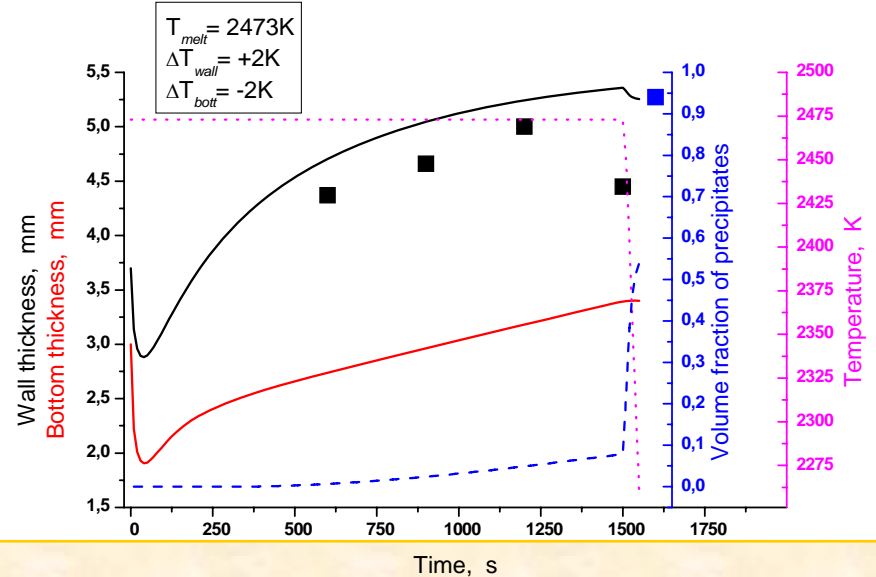
Analysis of short-term FZK crucible tests



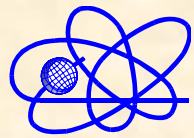
10 min.



20 min.



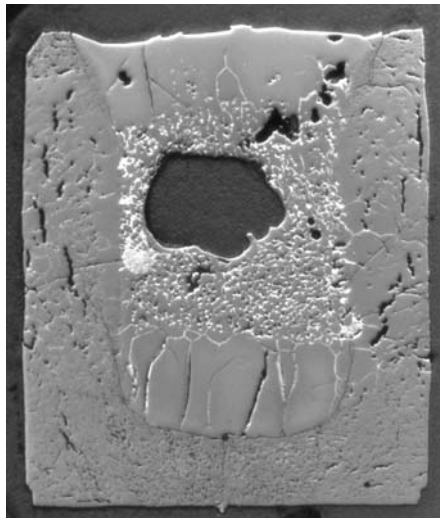
Analysis of long-term FZK crucible tests



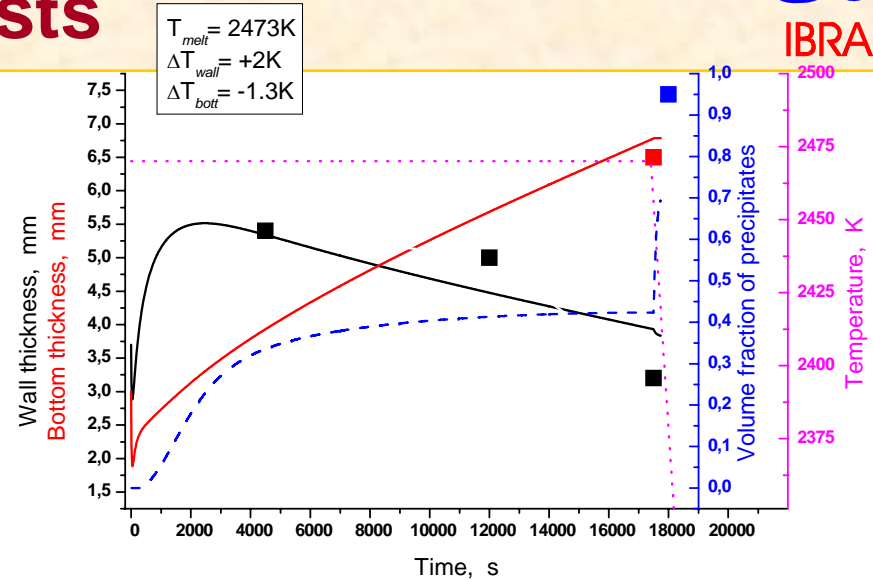
IBRAE



200 min.



290 min.



$$\frac{\lambda_{liq} \Delta T_{liq}}{2R} Nu = \frac{\lambda_{ox} \Delta T_{wall}}{d_{wall}}$$

$$R \sim 3.5 \text{ mm}, d \sim 7 \text{ mm}, \lambda_{liq} \sim 37 \text{ W/m}\cdot\text{K},$$

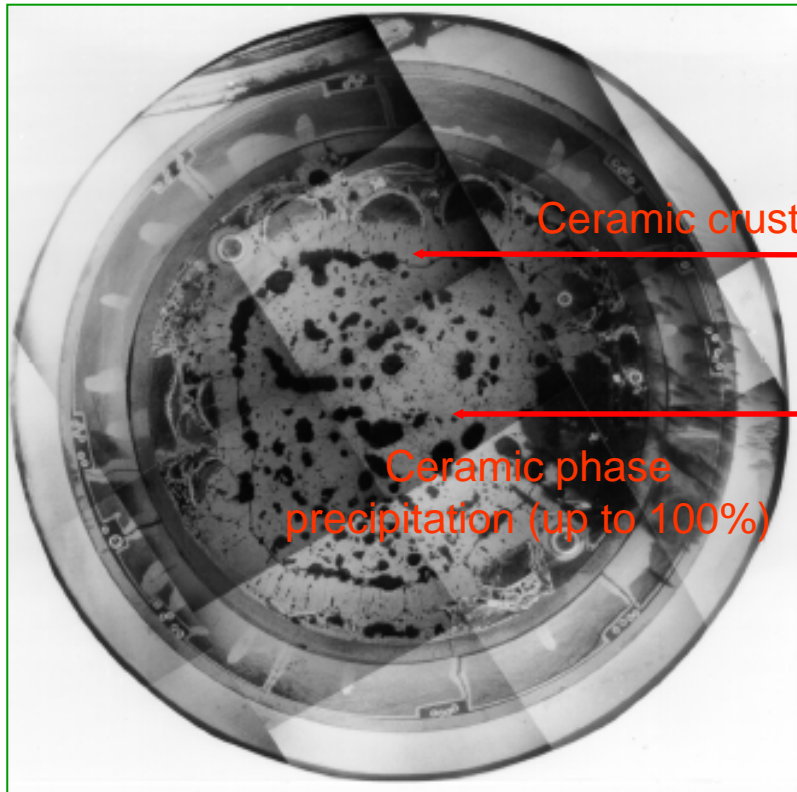
$$\lambda_{ox} \sim 1 \text{ W/m}\cdot\text{K}, Nu \sim 3,$$

$$\Delta T_{wall} \sim 50-100 \text{ K} \Rightarrow \Delta T_{liq} \sim +1 \text{ K}$$

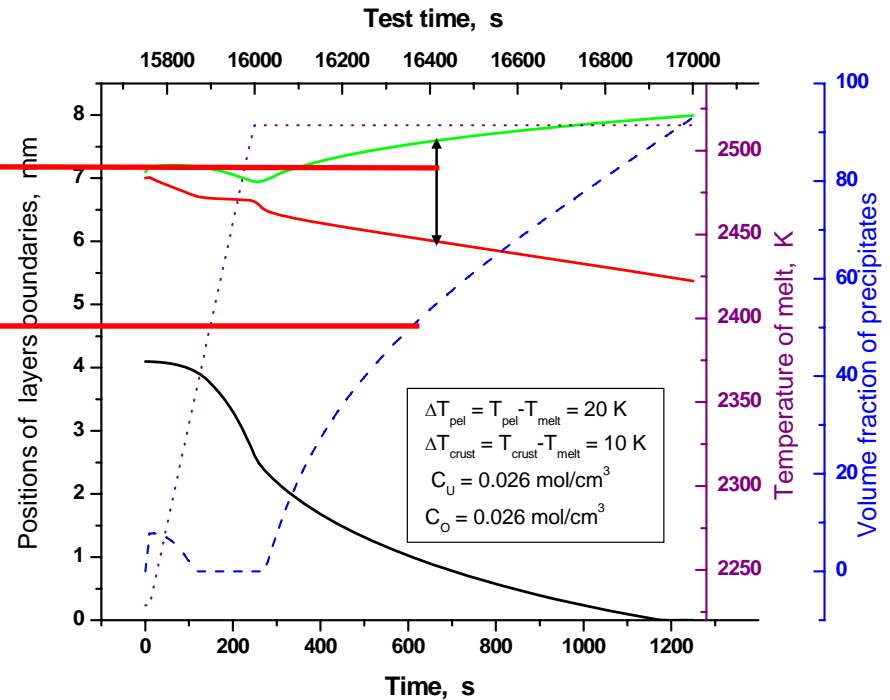
Conclusion: Oxide growth on “hot” oxidizing lateral walls was suppressed in expense of oxide growth on “cold” non-oxidized (!) free surface of melt (+ heavy precipitation in the melt)

Interpretation of melt oxidation in Phebus FP tests

Intensive dissolution of fuel rods and oxidation of molten pool up to complete conversion into ceramic phase

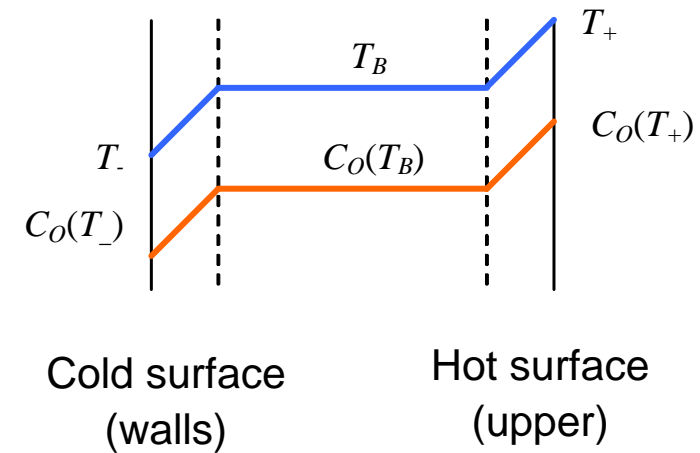
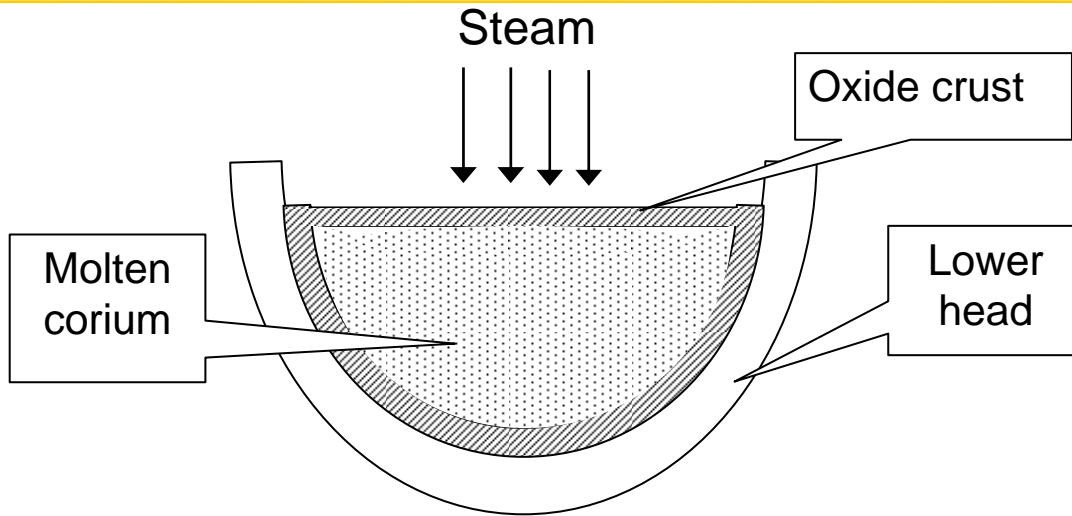


Post-test macrograph of (U,Zr)O₂ ceramic corium (molten pool)



Evolution of molten pool layers during transient

Molten pool oxidation in lower head of reactor vessel (1/3)



- Analysis of heat flux matches at the MP surfaces shows that temperature drop across the boundary layer in the melt is:
 - positive on the free upper surface, if heat losses from the surface are less in comparison with oxidation heat generated at this surface;
 - negative on crucible/melt interfaces owing to high heat losses in the cooled walls.
- After relatively quick attainment of melt saturation, a non-zero positive oxygen flux into the melt will persist on the oxidised (upper) surface and will be compensated by a negative oxygen flux from melt to the walls, resulting in oxide crust growth on the internal surface of the walls

Molten pool oxidation in lower head of reactor vessel (2/3)

Steady state consideration:

Wall:

$$W = \frac{\lambda_{melt} \Delta T_{melt}}{2R} Nu = \frac{\lambda_{ox} \Delta T_{ox}}{d_{ox}} = \frac{\lambda_{wall} \Delta T_{wall}}{d_{wall}}$$

$$T_{melt} \approx 2.5 \cdot 10^3 K, \Delta T_{wall} \approx 1.5 \cdot 10^3 K, \Delta T_{ox} \approx 0.8 \cdot 10^3 K,$$

$$Nu \sim 2 \cdot 10^3, R \sim 2 m, \lambda_{melt} \sim 37 W/m \cdot K, \lambda_{ox} \sim 2 W/m \cdot K,$$

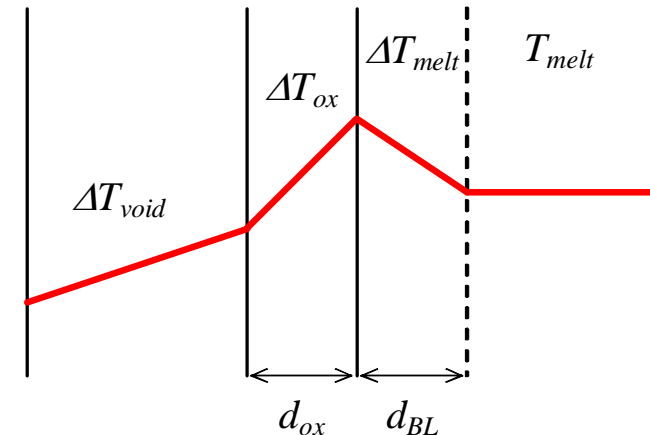
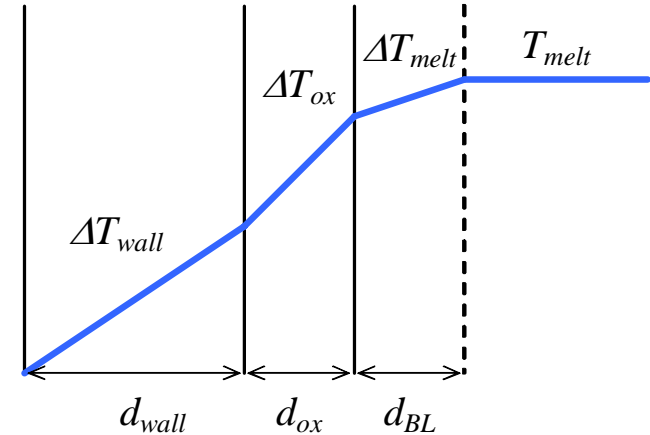
$$\Rightarrow \Delta T_{melt} = \frac{\lambda_{wall} \Delta T_{wall} \cdot 2R}{d_{wall} \cdot \lambda_{melt} Nu} \approx -60 K,$$

$$d_{ox} = \frac{\lambda_{ox} \Delta T_{ox} \cdot d_{wall}}{\lambda_{wall} \Delta T_{wall}} \approx 0.1 \cdot d_{wall}$$

Oxide crust:

$$\frac{\lambda_{liq} \Delta T_{crust}}{H} Nu + h(T_{ox} - T_0) = \dot{Q}_{ox}, \dot{Q}_{ox} \sim (1.5 \div 2.5) \cdot 10^5 W/m^2,$$

$$h(T_{ox} - T_0) \sim (0.5 \div 1.5) \cdot 10^5 W/m^2, \Rightarrow \Delta T_{melt} \approx +10 K$$

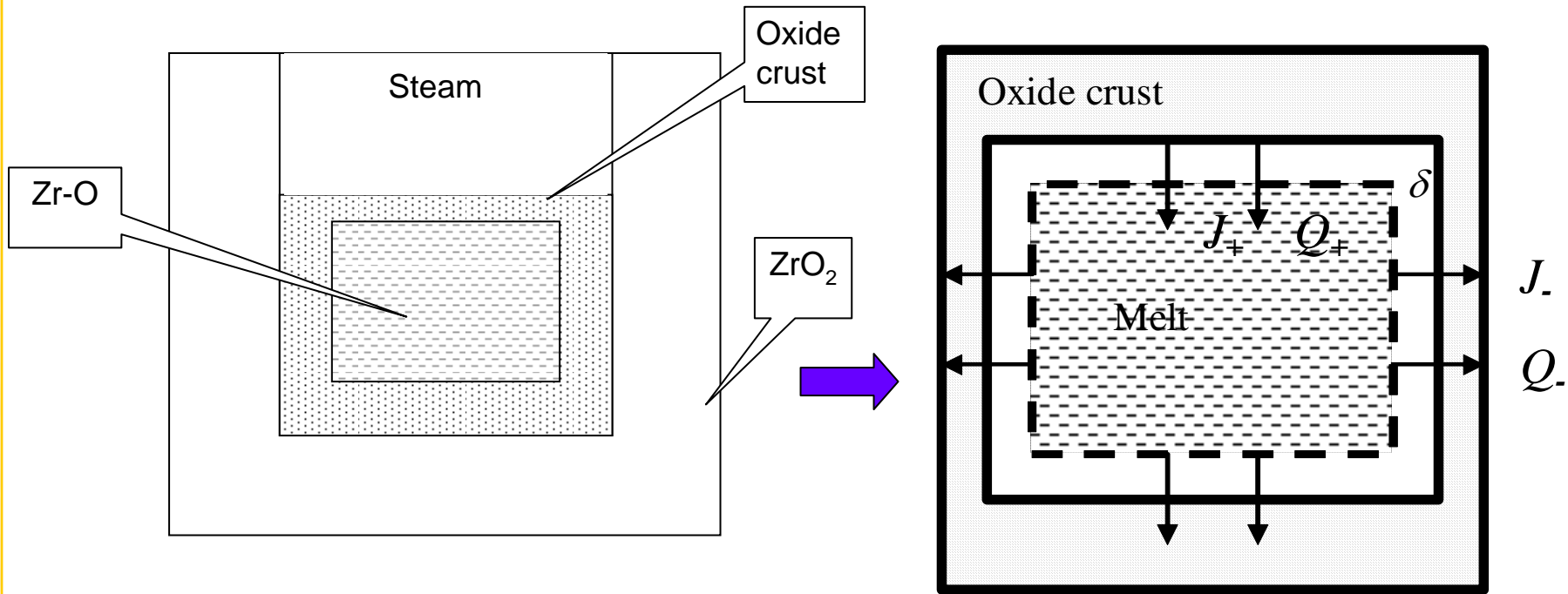


Model predictions

- In oxidizing atmosphere the oxide crust growth will take place on internal side of the walls accompanied with (possible) precipitation of ceramic phase in the melt bulk.
- After relatively quick attainment of steady-state conditions with oxide crust thickness of several mm ($\approx 0.1 d_{wall}$):
 - cooling of the MP through walls can be significantly suppressed;
 - the MP temperature will further increase;
 - possible corrosion (oxidation) and/or melting of a thin metal layer at the interface between the oxide crust and the wall can occur.
- To verify these predictions the new 2-d MP oxidation model was applied to simulate melt oxidation behaviour in simplified crucible tests (a possibility of such tests conductance is under discussion with FZK and KI).
- In the lack of detailed thermal hydraulic consideration, the main model predictions can be extended to large scales (RPV) only qualitatively.

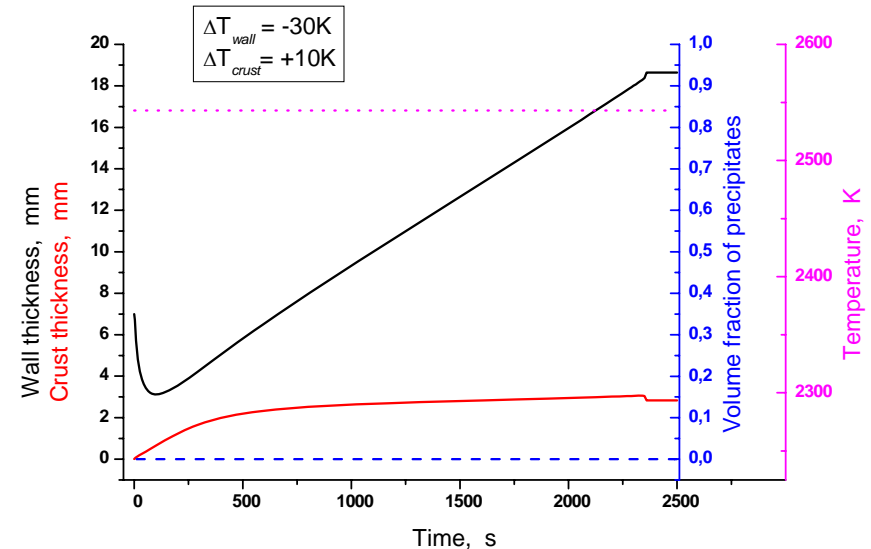
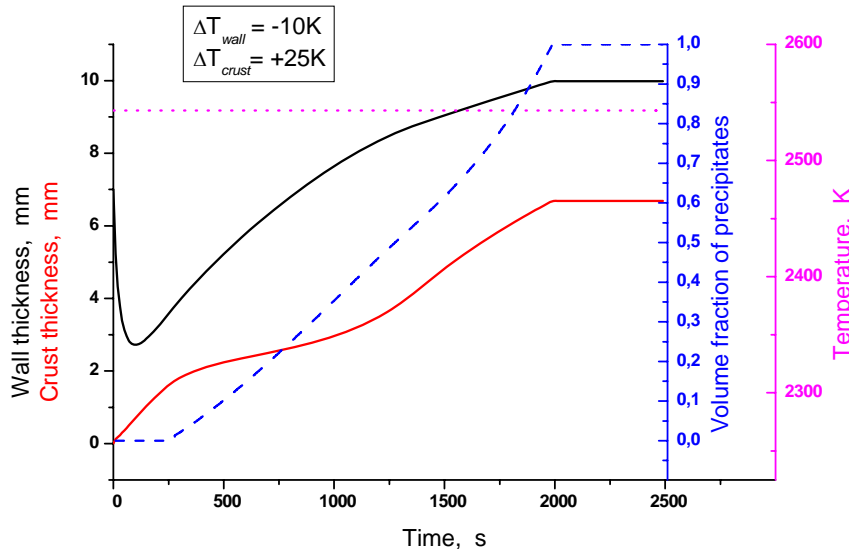
Simulation of molten pool oxidation in crucible tests (1/3)

Proposed crucible isothermal tests with “cold” ceramic walls and “hot” free oxidizing surface with inductive heating of metallic melt should model molten pool (MP) oxidation in the lower head of the (cooled) reactor vessel



Simulation of molten pool oxidation in crucible tests (2/3)

2-d model predictions for “cold” ceramic walls ($\Delta T_w < 0$) and “hot” free surface ($\Delta T_{up} > 0$) at the MP temperature 2540K

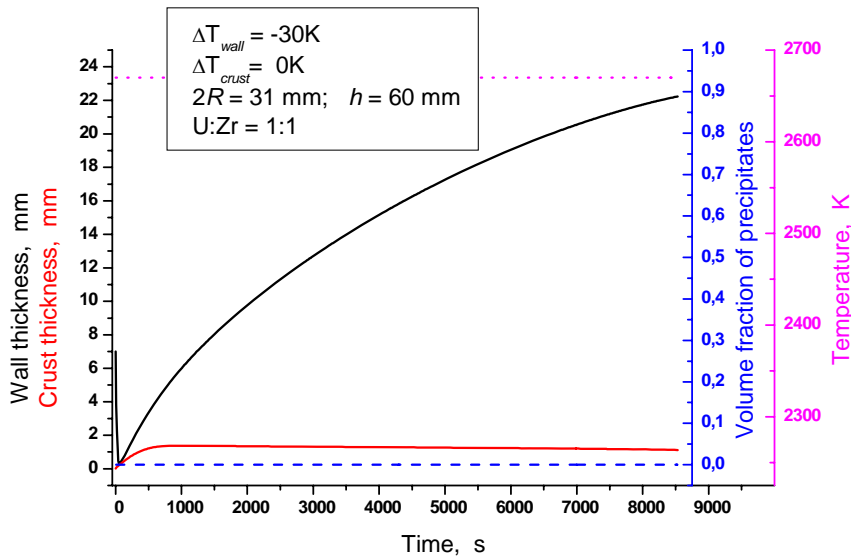


ZrO₂ crucible parameters: $R = 36.5$ mm, $h = 10$ mm, wall thickness 7 mm.

Charge is produced from the mixture of metallic Zr and ceramic ZrO₂ phases with the average atomic composition Zr:O = 2.7:1.

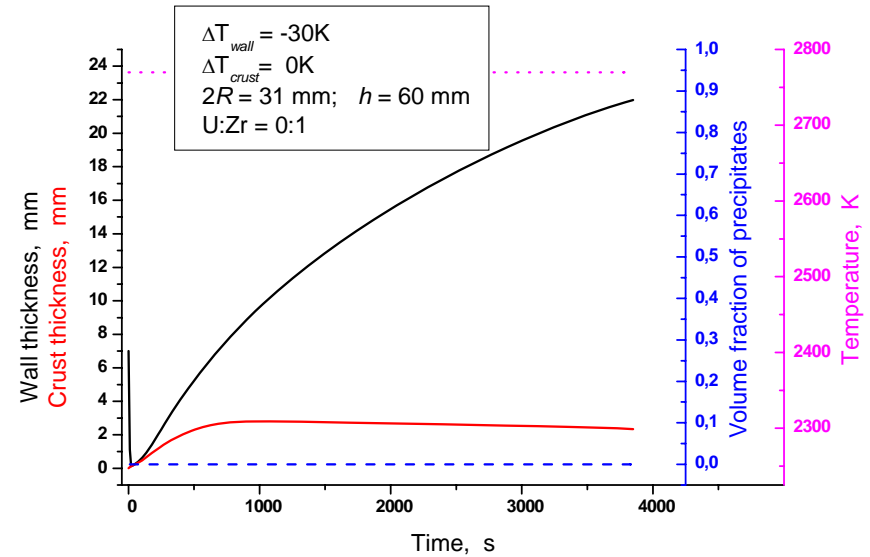
Simulation of molten pool oxidation in crucible tests (3/3)

- Large crucible
- U-Zr-O melt
- $\Delta T_{up} = 0$



Complete oxidation: $\approx 8000 \text{ s}$

- Large crucible
- High temperature (2770K)
- $\Delta T_{up} = 0$



Complete oxidation: $\approx 4000 \text{ s}$

Conclusion: owing to quick stabilisation of oxide crust thickness at the melt/steam interface, the total kinetics of melt oxidation obeys a (close to) linear (rather than parabolic) time law

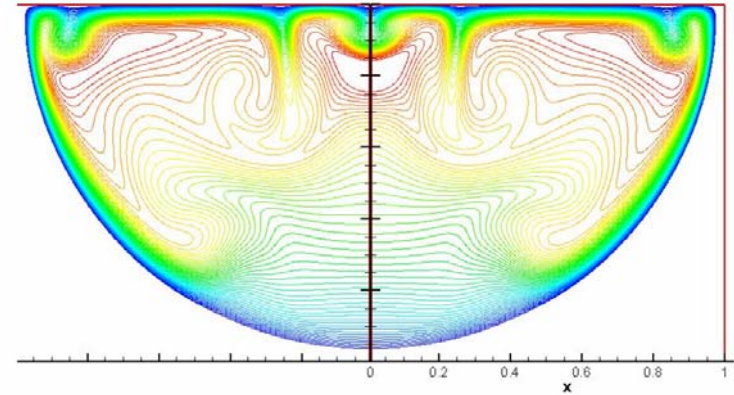
3-d CONV code developement

Main results from ISTC Project #2936

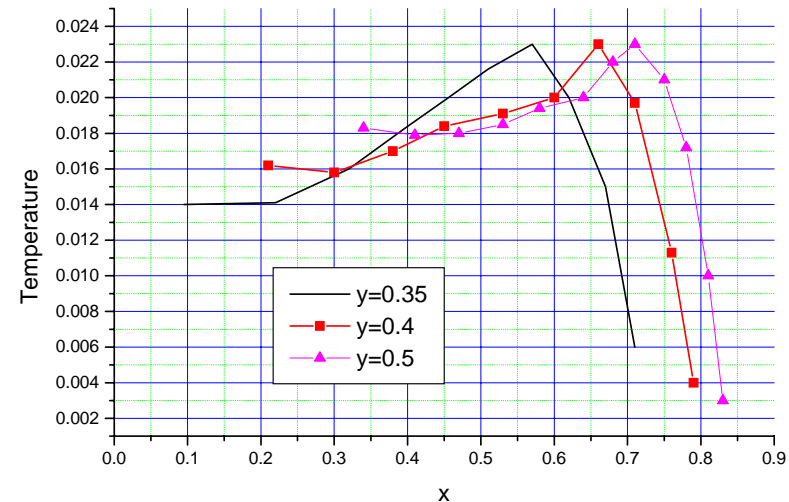
- 3D unified thermal hydraulic technique for simulation of multiphase processes in complex domains of convectively stirred melt in a wide range of parameters ($Ra < 10^{16}$ and $Re \approx 10^3-10^4$)
- DNS (Direct Numerical Simulation) and LES (Large Eddy Simulation) modelling approach to turbulent flows in the large-scale thermal hydraulic problems
- Simulation of phase changes in pure materials and binary alloys validated against tests on pure gallium melting
- Extensive validation against experimental data, including experiments with a heat generating fluid such as LIVE, COPO, SIMECO

Numerical predictions

Isotherms



Temperature profile. $Ra=10^{10}$



Conclusions (1/2)

- The advanced physico-chemical model for molten pool oxidation (coupled with the fuel pellet dissolution model) under non-equilibrium conditions of SA was developed in the SVECHA code within the ISTC Project #2936 in collaboration with European partners of the SARNET Project (JRC/IE, FZK).
- The main deficiency of the SVECHA approach is oversimplification of the thermal-hydraulic description of the convectively stirred melt. Similarly to modelling of crucible tests, the main thermal hydraulic characteristics of the convectively stirred melt were taken into consideration using simple correlations for the mass transfer coefficients at the oxide/melt interface.

Conclusions (2/2)

- The 3-d thermo-hydraulic code CONV initially designed in the frameworks of RASPLAV and MASCA Projects was strongly advanced in the ISTC Project #2936 for simulation of multiphase processes in complex domains of convectively stirred melt. The code already includes simplified models for simulation of phase changes and micro-segregation in binary alloys and is ready for implementation of more advanced physico-chemical models.
- Therefore, kinetics of molten pool oxidation which is of paramount importance with respect to core degradation and reactor pressure vessel failure analysis can be adequately modelled in multi-scale approach (crucible → bundle → reactor) by tight coupling of the SVECHA physico-chemical model with the thermo-hydraulic code CONV.