**Main results of the ISTC Project #3876 “Thermo-Hydraulics of U-Zr-O Molten Pool under Oxidising Conditions in Multi-Scale Approach (Crucible - Bundle - Reactor Scales)”, (THOMAS)**

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# *ABSTRACT*

*Main results of the ISTC Project #3876, performed in 2009-2011, are presented. The new physico-chemical model of corium melt oxidation and interactions with vessel steel, verified against METCOR tests observations, is implemented in the thermal hydraulic code CONV2D and applied to consideration of the reactor pressure vessel (RPV) failure under conditions of interactions with U-Zr-O corium melt and external wall cooling by water.*

# Introduction

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 were observed at upper elevations in bundles in the early stage of core degradation in CORA [1, 2] and QUENCH tests [3, 4]. Results of the Phebus FP tests [5, 6] confirmed that a significant part of the fuel bundle was liquefied and that the amount of fuel damage was close to TMI-2 [7] with an extended molten pool located in a central zone of the bundle underneath a cavity. In the late stage of a severe accident, melt can relocate into the lower head of the reactor pressure vessel and form a large molten pool interacting with cooled walls. The details of in-vessel melt pool behaviour are preconditions for possible in-vessel melt retention considerations. The in-vessel melt retention aspects and the improvement of the predictability of the thermal loading are a matter of especially high interest and a priority for BWR and reactors with low power density (e.g. VVER-440), but also for large PWR and VVER reactors [8].

Oxidation kinetics of Zr-containing melts can be significantly higher in comparison with that of solid materials, therefore, it largely determines the high heat generation and hydrogen source term during severe accidents, as unambiguously shown, e.g., in the QUENCH tests [3, 4]. On the other hand, the oxidation kinetics strongly depends on thermal hydraulic behaviour of oxidized melt. Therefore, there is a critical need to investigate the in-vessel molten pool behaviour under oxidation conditions and to predict the changes corium will undergo, including the main phenomena, which can govern these changes: natural convection in the molten pool; corium oxidation including H2 production; dissolution and/or corrosion of reactor vessel steel.

Oxidation kinetics of Zr melt was initially investigated at FZK in small-scale crucible tests [9]. Qualitative results of those studies allowed better understanding and interpretation of corium oxidation in CORA and QUENCH tests. Within the previous ISTC Project #2936 a significant effort was undertaken for the development of numerical physico-chemical model for the U-Zr-O melt oxidation and relocation [10]. Being developed on the base of the crucible tests, the new model was extended later to a larger scale and allowed quantitative interpretation of observations from CORA, QUENCH and Phebus tests ("molten pool oxidation"). The model development was initiated in the frames of the COLOSS Project (5th FP) [11, 12] whereas its implementation in the SVECHA code and application to the bundle tests [13, 14] were strongly supported by SARNET NoE (6th FP) in collaboration with JRC/IE and FZK.

The main deficiency of the SVECHA approach was the simplified thermal-hydraulic description of the convectively stirred melt. Similarly to modelling of crucible tests, in this approach the main thermal-hydraulic characteristics of the convectively stirred melt were taken into consideration in the form of simple correlations for the heat and mass transfer coefficients at the oxide/melt interface. However, such important predictions of the new model for the melt interacting (at its open surface) with steam as formation of a thick oxide crust on cold walls (owing to oxygen transport from the open surface to the walls through the convectively stirred melt under non-equilibrium temperature conditions) which can essentially suppress corium coolability, require more detailed and self-consistent consideration of mass- and heat-exchange processes in the melt, especially in the prototypic (large-scale) geometry of the reactor pressure vessel. These important phenomena can be adequately modelled only by tight coupling of the physico-chemical melt oxidation model with advanced thermal-hydraulic codes.

In parallel, the 2D and 3D unified thermal-hydraulic technique for simulation of multiphase processes in complex domains of convectively stirred melt were strongly advanced in the CONV code within the same ISTC Project #2936. Initially developed in the framework of RASPLAV and MASCA Projects [15, 16], the code was further improved and validated in the ISTC Project using experimental data, including experiments with a heat generating fluids like LIVE, COPO, SIMECO [17, 18]. Numerical approach and computing module for simulation of phase changes in pure materials and binary mixtures were developed and tested against melting of pure gallium [19].

For multi-dimensional simulation of various thermal-hydraulic processes in NPP in a wide range of parameters (Ra < 1016 and Re ≈103-104) the 3D unified CFD numerical technique was developed. Results of numerical testing in the area of turbulent flows allow a possibility of DNS (Direct Numerical Simulation) and LES (Large Eddy Simulation) modeling approach to the large-scale thermal hydraulic problems [20].

The ISTC Project #3876, performed at IBRAE in collaboration with IRSN, CEA, KIT, ITU and IVS (Trnava) under supervision of CEG-SAM, was aimed at the tight coupling of the two advanced tools developed within the previous Project #2936: the SVECHA physico-chemical (molten pool oxidation) model and the thermo-hydraulic code CONV. This allowed a realistic mechanistic description of U-Zr-O molten pool behaviour in oxidizing conditions and extended the thermal hydraulic consideration of oxidized melt from small scale (crucible tests) up to a large scale (reactor pressure vessel), including an intermediate scale corresponding to molten pools in the bundle tests. For further application of the melt oxidation model to the case of U-Zr-O corium molten pool confined by steel walls cooled outside (e.g. pressure vessel walls), the model was generalised to consideration of (oxidised) corium interactions with the walls, leading to strong corrosion and thinning of the walls.

# Model for oxidised corium melt interactions with vessel steel

The model for corium melt oxidation under non-equilibrium conditions (characterised by temperature difference between liquid and solid phases) is extended to consideration of U-Zr-O corium melt interactions with steel walls (in the geometry of the pressure vessel, Figure 1), by introduction of additional terms in the mass and heat flux matching equations formulated in [15].



Figure 1: Schematic representation of the molten pool geometry.

In order to describe local interactions at the corium-steel interface, taking into account that temperature and concentration gradients along the interface can be generally neglected in comparison with those in the perpendicular direction, a 1d approach (in perpendicular, or radial direction for each calculation mesh) can be used. This allows the above-described melt oxidation model to be reduced to simplified 1d consideration, on the one hand, and coupling of the model with the thermal-hydraulic code (for more adequate consideration of heat and mass exchange with the melt).

As a result, the 1d physico-chemical interactions model simulates evolution of the solid phase layers in each mesh: (Zr,U)O2-x crust (formed in a steep temperature gradient near the interface), FeO corrosion layer and steel wall, as well as temperature distributions in the layers, heat and U, Zr, O molar fluxes into the melt, Figure 2.

1d oxygen transfer in the (Zr,U)O2-x crust is simulated by numerical solution of the partial derivative diffusion equation for the oxygen concentration  in various interaction layers with moving boundaries. The oxygen boundary concentrations are determined using the equilibrium U-Zr-O phase diagram. Relocation of boundaries between various layers is calculated by matching oxygen and heat fluxes at the interfaces. Steel surface oxidation is simulated by the parabolic correlation for the weight gain, if the calculated oxygen flux from the (Zr,U)O2-x crust is sufficient. In the opposite case, FeO oxide weight gain is controlled by the oxygen flux from the crust (Section 2.1). At higher temperatures, manifested by eutectic interactions at the crust-oxide interface, a more complicated (“flowering”) mechanism is introduced for description of accelerated corrosion kinetics (Section 2.2).

Conversion (to solid) and growth of the mushy crust in steep temperature gradient can be examined with the new analytical model [21] based on the Flemings-Brody approach, which can be numerically realized after coupling of the interaction model with a thermal hydraulic code. Solution of the heat- and mass-transfer equations with flux matches at the mushy-zone interfaces describes the emergence of the two-phase zone precisely under Mullins-Sekerka condition for the plane front instability. This reflects the self-consistency of the new model. Currently this effect is neglected (under assumption of rapid conversion of the mushy zone into ceramic layer in oxidized melt) and crust is considered as a solid layer.



Figure 2: Schematic representation of the temperature and concentration distribution in 1d model.

## Steel corrosion model (low temperatures)

Corrosion of steel walls is analyzed using experimental data for 15 Kh2NMFA vessel steel from METCOR tests [22]. The model for steel corrosion based on the measured parabolic correlation

, (1)

is supplied with the “oxygen starvation” regime consideration, in which steel oxidation kinetics is controlled by external oxygen flux. The starvation regime occurs during relatively long period of corrosion when the corrosion layer is relatively thin (in comparison with the crust), thus, transport of Fe and/or O ions through this layer is a relatively rapid process and its growth is controlled by the oxygen supply from the (solid or mushy) crust (calculated by the diffusion transport model above described), .

Therefore, an additional equation for variation of the FeO layer thickness  takes the form

, (2)

if calculated  is smaller than  derived from Eq. (1),  (i.e. in the starvation regime); otherwise, in the parabolic regime

. (3)

For simplification, only FeO corrosion layer is considered in the model, neglecting its difference with Fe2O3 (or Fe3O4) layers, which are notably thinner than FeO layer [22].

It should be noted that the rate-controlling process of steel corrosion kinetics in oxidizing atmosphere (under unlimited oxygen supply) is iron (Fe2+) diffusion through the layers. However, as mentioned above, the rate control can be violated in the case of the corrosion layer growth under restricted oxygen supply induced by the adjacent crust layer (i.e. in the oxygen starved regime).

This conclusion can be confirmed by a remarkable dependence of the corrosion rate on the oxygen potential in the melt revealed in METCOR tests. In particular,lower corrosion rate measured in some of the tests correlated with insufficient air supply to the melt and decreased oxygen potential of the melt. A similar qualitative conclusion can be derived from tests [23], where it was demonstrated that the zirconia coatings deposited on steel substrate strongly retarded the steel oxidation, and the oxidation rate decreased with increasing coating thickness (from 1 to 6 layers of ≈ 40 nm thickness). Furthermore, iron diffusion through the (U,Zr)O2 crust is assumed to be a rather slow process, based on experimental evidence of extremely low Fe diffusivity in ZrO2 [24], thus, oxygen diffusion is considered as the mass transport mechanism in the (U,Zr)O2 crust.

For these reasons, the developed model is essentially based on consideration of oxygen transport through the interaction layers, which is self-consistently combined with consideration of Fe ions diffusion through the (oxide) corrosion layer (by consideration of Fe+ diffusion as the rate controlling step, represented by the parabolic kinetics, Eq. (1), under normal, non-starved corrosion conditions). The model allows interpretation of the main tests observations and qualitatively correctly describes vessel steel corrosion kinetics observed in low-temperature regimes of METCOR tests (see Section 2.3). However, for high temperatures, when a molten (eutectic) phase appears at the crust-oxide interface, a more complicated model is required.

## Steel corrosion model (high temperatures)

At high temperatures characterized in METCOR tests by > 1300°C and manifested by eutectic melt formation at the interface between corrosion FeO and crust (U,Zr)O2 layers, accelerated steel corrosion kinetics was observed in the tests. Since the eutectic temperatures are very close in both equilibrium pseudo-binary FeO-ZrO2  and FeO-UO2  phase diagrams, ≈ 1600 K, the same temperature criterion can be assumed also for the mixed oxide (U,Zr)O2 interface with FeO, ≈ 1600 K.

Indeed, under low temperature conditions (with  < 1600 K at the oxide-crust interface) when eutectic liquefaction of FeO apparently did not take place, its thickness roughly corresponded to the corrosion depth (see Figure 3 taken from [22]). In the case of high > 1600 K, when FeO phase was liquefied owing to eutectic interactions with the crust, the corrosion depth attained ≈ 5 mm, whereas only a very thin corrosion layer (of ≤ 200 μm) was retained in-between steel and the crust (see post-test Figure 4 taken from [25]). Simultaneously, the presence of tree-like branching cracks in the crust typical of a stress regime was observed, see Figure 4.

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| Figure 3: Morphology of the corium–steel interaction zone in MC-2 test. I: initial position of specimen surface. (1) Steel specimen; (2) FeO corrosion layer, (3) Fe2O3 corrosion layer, (4) crust (from [22]). | Figure 4: Microstructure of interface between steel (lower, grey layer) and (U,Zr)O2 crust (upper, white layer) in MCP-2 test (from ([25]). |

The accelerated corrosion kinetics can be described in the current approach using “flowering” mechanism, which was developed earlier for interpretation of ZrO2 shell failure above Zr melting point [26], observed in the high-temperature tests on fuel rods degradation under oxidizing conditions [27]. Following this mechanism, it is assumed that, owing to volumetric expansion of oxidized steel confined by the solid crust, high tensile stresses are induced in the crust leading to its cracking and/or tearing, see Figure 5. This conclusion is general either for low-temperature conditions or for high-temperature conditions, however, with some important differences. Indeed, at low temperatures (below FeO-crust eutectics formation) corium melt penetrates into tears or cracks, immediately freezes and thus heals them over, whereas at high temperatures eutectic melt is extruded into the tears/cracks (owing to high compressive stresses in eutectic melt) and eventually penetrates into the corium.

This extrusion (or drainage) of eutectic melt provides rather small mean thickness of the eutectic layer during corrosion process, which in calculations can be neglected in the first approximation, in a qualitative agreement with observations in Figure 4. As a result, corrosion depth grows up with an increased rate, as will be demonstrated in the next Section.



Figure 5: Schematic representation of the flowering mechanism.

## Numerical simulations

The new model was numerically realized and applied to consideration of typical temperature scenarios of METCOR tests (MC-10 and MCP-2) with U-Zr-O corium [25]. Since step-wise temperature scenarios (including various temperature plateaus) were maintained in these tests, comparison of post-test measurements with the model predictions is not straightforward and thus was not attempted. For this reason, only semi-quantitative comparison of calculation results (for simplified temperature scenarios with one plateau) with online measurements at various temperature plateaus were carried out. However, these model predictions can be directly compared with results of future tests with simplified, one-plateau temperature scenarios, which seem rather important for reliable verification of models and are recommended for future implementation.

Two typical scenarios, low-temperature (< 1600 K) and high-temperature (> 1600 K), were considered in simulations. Temperature of 70% UO2 – 30% ZrO2 melt (mass %) was fixed at 2800 K, whereas temperature of the steel outer surface (< 373 K) was chosen to maintain predetermined conditions, , at the inner (interacting) surface of steel. Calculated (under these boundary conditions) temperatures at the crust-FeO interface, , and the mean temperatures of the crust, , are presented in Figure 6.

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| Figure 6: Low-temperature, < 1600 K (*left*), and high-temperature, > 1600 K (*right*), scenarios of two calculation runs. | |

Results of calculations under these temperature conditions for corrosion depth and thicknesses of the crust and steel oxide (FeO) layers are presented in Figure 7. In the low-temperature case (left panel of Figure 7) the oxide layer thickness is small (≤ 0.5 mm) and roughly corresponds to the corrosion depth, in a qualitative agreement with observations (see Figure 3), whereas the crust thickness is relatively thick (owing to a large temperature drop across this layer). Under these conditions the calculated steel surface temperature in the steady stage is ≈ 1200 K, the heat flux is *F* ≈ 1 MW/m2 and the corrosion rate attains *R* ≈ 0.1 mm/h, in a reasonable agreement with online measurement evaluation in regime 1 of MCP-2 test (*R* ≈ 0.085 mm/h at ≈ 1140 K and *F* ≈ 0.74 MW/m2).

In the high-temperature case (right panel of Figure 7), the corrosion rate attains *R* ≈ 5 mm/h at *TS* ≈ 1800 K and *F* ≈ 1.5 MW/m2, that fairly corresponds to online measurement evaluation in regime 9 of MCP-2 test (*R* ≈ 5.8 mm/h at ≈ 1640 K and *F* ≈ 1.2 MW/m2).

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| Figure 7: Calculation results for two temperature scenarios from Figure 6, < 1600 K (*left*) and > 1600 K (*right*). | |

As a result, the model predicts that the corrosion of steel in contact with oxidised corium becomes a rather critical factor for the cooled vessel integrity, if the temperature at the oxide-crust interface exceeds the eutectic point of ≈ 1600 K. Indeed, calculation results for typical values of the heat and oxygen fluxes in the molten pool geometry (from Figure 1), presented in Figure 8, demonstrates significant corrosion effect during periods of molten pool retention in the lower head vessel typical for severe accidents.

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| Figure 8. Calculation results for variation of steel vessel wall thickness with time in the molten pool geometry from Fig. 1 (r1 = 2.0775 m) at > 1600 K (outer surface temperature – 273 K) at fixed heat flux from the melt - 2×105 W⋅m-2 (*left*) and at fixed oxygen flux from the melt – 0.5 mole⋅m-2⋅s-1 (*right*). | |

As seen from this figure, corrosion thickness is rather sensitive to the values of heat and oxygen fluxes from the melt. For this reason, self-consistent calculation of wall corrosion will be possible after coupling of the current melt oxidation-steel corrosion model with the thermal hydraulic code CONV2D. Results of such calculations will be presented in Section 4.

# Thermal-hydraulic code conv2d

For numerical simulation of convection/diffusion processes with regard to a melt and melt retention in the reactor vessel, the two-dimensional and three-dimensional software (computer codes CONV2D and CONV3D) was developed.

While developing the codes, attention was mainly paid to the computational hydrodynamics, namely to the numerical techniques for solving two and three-dimensional Navier-Stokes and energy equations. An important particularity of these codes is an account of phase transitions such as melting and solidification. In other words, computer codes were developed for solving a system of Navier-Stokes equations utilizing Boussinesq approximation and equations for energy with varying coefficients  and constant  and  in rectangular and semicircular domains in a wide range of Rayleigh number . Similar requirements were stipulated in the first place by peculiarities of RASPLAV experiments [15], in the support of which the CONV code was originally developed.

CONV code allows out calculations to be carried out in various geometries from most simple (rectangular, semicircular) up to complex constructional features of experimental facilities. The calculations can be performed under various boundary conditions, with various materials. Results obtained by CONV code can be presented as the graphs and are saved as rigid copies with tools available for a user, and using a visualization system designed in support of the code. CONV code was validated against a wide set of experimental and benchmark tests [28].

## Basic equations

The momentum equation looks like

, (4) where  is the velocity vector,  is the convective operator (which for an arbitrary vector  can be written as ),  – pressure, normalized by density,  and  – viscosity and turbulent viscosity,  – gravity acceleration,  – thermal expansion coefficient, – temperature, – temperature of environment.

The energy equation looks like

, (5)

where  – density,  – specific thermal capacity,  and – heat conductivity and turbulent heat conductivity, respectively;  – thermal source.

The coefficients, right part and boundary conditions of the equation are initialized through input files.

For the oxygen transport the following equation is used

, (6)

where  – concentration,  and – diffusivity and turbulent diffusivity,  – concentration source. The coefficients, r.h.s. terms and boundary conditions of the equation are initialized through external function. In the current approach oxygen is considered as a passive impurity, which does not influence the melt density. In the subsequent development of the code it is foreseen to take oxygen into consideration as an active impurity, influencing the melt convection. The oxygen turbulent diffusivity  is calculated in the Detached Large Eddy Simulation (DLES) approach (see below).

## Turbulence models

CONV code is modernized by inclusion of approximating turbulence model and QDNS approach. For improving turbulence modelling at extremely high Rayleigh numbers, LES approach was implemented in CONV code. Implementation was accompanied by numerical experiments for the choice of a set of commutative filters for the LES approach.

The numerical experiments for the choice of optimum turbulence model (algebraic type) were carried out. Among them are: 1) approximated turbulence model, 2) algebraic turbulence model (Bolduin-Lomax) and 3) quasi DNS approach (QDNS). The approximated turbulence model was proposed and calibrated for convection of a heat-generating fluid in a wide range of Rayleigh numbers from moderate up to extremely high.

For simulation of a turbulence stipulated by geometrical singularities, Detached Large Eddy Simulation (DLES) approach was realized, in which dynamics of large-scale eddies is calculated, while effect of a small-scale turbulence are simulated. The basic equations for large eddies are obtained by spatial averaging or application of procedure of filtration, which removes small-scale oscillation from the Navier-Stokes equations. For simulation of small-scale eddies the Smagorinsky’s model is used.

## Implementation of the melt oxidation/corrosion model in CONV2D

Implementation of the physico-chemical model for U-Zr-O melt oxidation and steel corrosion (as a stand-alone module HTLQ) into the code CONV2D was carried out. As a result, evolution of U-Zr-O corium melt temperature and composition distributions is calculated by the 2D thermal hydraulic code. The oxidation module is coupled with the 2D thermal hydraulic code through the heat and oxygen mass flux matching at the melt-solid interface. Additionally, bulk concentrations of the melt components (U, Zr, O) and temperature of the melt in the boundary thermo-hydraulic spatial mesh are inputs for the 1D HTLQ module. The oxidation module is called for each thermo-hydraulic spatial mesh at the melt-solid interface.

Furthermore, the solution block of an advection-diffusion for oxygen in CONV2D was improved and adaptation of turbulence model in CONV2D for solving oxygen transport problem in the reactor case was carried out. Extension of the thermal hydraulic consideration of oxidized melt and its interaction with the vessel steel walls from small scale (crucible tests) up to a large scale (reactor pressure vessel) was carried out.

# calculation results

Coupled CONV2D-HTLQ code (2d thermal hydraulic code CONV2D and 1d oxidation module HTLQ) was initially used for calculations of steel vessel corrosion with the molten pool in geometry similar to that represented in Figure 1 (half ellipse), however, of small size. Namely, internal radius of the crucible at the top was r1 = 0.04 m, vertical dimension of melt corium – 0.04 m, steel wall thickness – 60 mm, number of nods for the melt convection simulation was 513 × 513. Heat source was in the range 103 - 104 W, oxygen flux — 0.5 - 1 mole⋅m-2⋅s-1 at the top surface of the melt corium. Initial temperature of the melt was 2673 K, outer surface temperature - 1300ºC (to avoid melt cooling down in calculations), and initial oxygen concentration in the melt corium was 105 mole⋅m-3. Time step of thermo-hydraulic code calculations was in the range 2⋅10-2 – 0.1 s.

Calculations for distribution of temperature, vertical velocity and oxygen in molten corium pool during initial moments of interactions (5 and 35 s) are presented in Figure 9. Calculations show that notable stratification of temperature in the melt is attained rather rapidly, whereas penetration of oxygen from the upper (oxidized) surface to the melt bulk through the boundary layer is a relatively slow process.

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| 5 s | 35 s |
| Figure 9: Calculation results for distribution of temperature (*upper part*), vertical velocity (*middle part*) and oxygen (*lower part*) in the oxidized melt owing to free convection in the small-scale reactor pressure vessel geometry during initial 5 s (*left*) and 35 s (*right*) | |

The coupled code was further applied to calculation of vessel steel interactions with molten corium in a more realistic geometry represented at Fig. 1 (half ellipse) with melt volume 6.8 m3. Internal radius of the vessel at the top was r1 = 2.0775 m, vertical dimension of melt corium – 2.3 m, steel wall thickness – 190 mm, number of nods for the melt convection simulation were 1025×1025. The heat source in the melt was chosen as 8×105 W, conservatively corresponding to a relatively late stage of decay heat in the melt (≈0.1 W/m3). Temperature boundary conditions in the calculations were: constant temperature at the outer surface of steel wall 373 K (corresponding to the convective boiling regime); zero heat flux from the top surface of the melt corium. Boundary conditions for oxygen were: zero oxygen flux at the outer surface of steel wall, and oxygen flux 1 mole m-2 s-1 at the top surface of the melt corium. Initial temperature of the melt was 2773 K, and initial oxygen concentration in the melt corium was 105 mole m-3.

The cooling of the RPV outside vessel wall with water during a severe accident with a core melt down is believed to be an effective method to stabilize the vessel and prevent vessel failure, which are to be studied in the current calculations.

Calculations were performed in two steps: first 1000 time steps at the initial stage after initialization of thermo-hydraulic conditions only CONV2D module calculates (it took approximately 9 hours in Intel Core 2 Duo 2.53 GHz), and then using restart file coupled calculations with CONV2D-LQHT code were performed during 104 time steps (it took approximately 50 hours in Intel Core 2 Duo 2.53 GHz). Time step of thermo-hydraulic code calculations was in the range 2⋅10-2 – 0.1 s.

Calculation results for the melt temperature (near the wall) and steel temperature (at the interface), and for crust and wall thicknesses are presented at Fig. 10. From these figures it is seen that, owing to oxygen redistribution in the melt (illustrated in Fig. 9), the solid crust formed near the vessel walls is chemically unstable at higher elevations and disappears within several minutes. This behavior is similar to the “corrosion-erosion” effect, observed by J. Stuckert in the FZK crucible tests [9], where growth (corrosion) or dissolution (erosion) of the oxide phase (walls of ZrO2 crucible) was controlled by the oxygen flux matches at the interface with the U-Zr-O melt [9, 13]. After crust dissolution, direct contact of melt with steel is attained, resulting in rapid thinning of the vessel wall up to a few mm thickness within 6-8 min at the upper (5°) and medium (45°) elevations. At the lower elevations (90°) the crust is stable, preventing vessel walls from the chemical attack by the corium melt. In this position only relatively slow wall thinning owing to steel corrosion is calculated.

These calculation results indicate, despite their preliminary character (some simplifications are still used), that in-vessel retention after relocation of corium into the lower plenum by cooling the outside vessel wall with water might be ineffective even in a late stage when decay heat is relatively small, ≈ 0.1 W/m3. This important conclusion suggests further, more thorough investigation of the physico-chemical stability of the ceramic crust that prevents vessel walls from direct attack of corium melt and failure.

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| Figure 10: Calculation results for: r1 = 2.0775 m, outer surface temperature - 100ºC, initial melt temperature – 2773 K, heat source - 8×105 W, initial oxygen concentration - 105 mole m-3, oxygen flux to the melt - 1 mole m-2 s-1. |

# Conclusions

The model for U-Zr-O molten pool oxidation (developed within the previous ISTC Project #2936) was updated for simultaneous consideration of vessel steel (VS) corrosion by the corium melt. The model allows interpretation of the METCOR tests observations and correctly describes VS corrosion kinetics observed in low- and high-temperature regimes in a qualitative manner. For description of accelerated VS corrosion kinetics observed in high-temperature regimes the new model using a “flowering” mechanism was developed and implemented in the corrosion model. After testing and verification, the new 1D physico-chemical interactions module HTLQ was prepared for implementation in the 2D thermal hydraulic code.

The thermal-hydraulic code CONV2D was significantly modified. In particular, the oxygen advection-diffusion block in CONV2D was developed. Adaptation of turbulence model for solving the oxygen transport problem in the reactor case and modification of the boundary conditions block for oxygen transport in CONV2D were carried out

Oxidation/corrosion module HTLQ was implemented in CONV2D; the coupled code was thoroughly tested and verified. results on convection mixing of oxidized corium and VS wall corrosion in simplified (small scale) geometry of RPV and for short initial period were obtained.

Calculation results indicate that in-vessel retention after relocation of corium into the lower plenum by cooling the outside vessel wall with water might be ineffective, owing to physico-chemical dissolution of solid ceramic crust, formed at the melt/wall interface and preventing vessel walls from direct attack of corium melt. This important conclusion suggests further, more thorough investigation of the crust stability under conditions of oxidized corium convection in RPV with residual heat generation in the melt and external wall cooling by water.

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