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| ISTC Project No. 3876 | | |
| “Thermo-Hydraulics Of U-Zr-O Molten Pool under Oxidising Conditions in Multi-Scale Approach (Crucible - Bundle - Reactor Scales)” | | |
| Annual Project Technical Report | | |
| on the work performed from October 1, 2009 to September 30, 2010 | | |
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| Title of the Project: | Thermo-Hydraulics Of U-Zr-O Molten Pool under Oxidising Conditions in Multi-Scale Approach (Crucible - Bundle - Reactor Scales) |
| Contracting Institute: | Nuclear Safety Institute of Russian Academy of Science (IBRAE) |
| Participating Institutes: |  |
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# Brief description of the work plan: objective, expected results, technical approach

The physical phenomena involved in severe accidents are extremely complex and generally demand the development of specific research, aimed to further understanding of these physical phenomena and to reduce the uncertainties surrounding their quantification. In this field, there is no way to conduct experiments on full scale and to reproduce all the possible situations. Therefore the ultimate goal is to develop models, which are validated on the basis of scaled experiments and which then can be applied to the reactor cases. These models, grouped together in computer codes, should allow predicting severe accident progression.

The Project aims 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 will allow a realistic mechanistic description of U-Zr-O molten pool behaviour in oxidising conditions and will extend the thermal hydraulic consideration of oxidised 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. Moreover, improved interpretation of Phebus FP tests observations of corium melt oxidation, as well as transposition of thermal hydraulic consideration from the experiments (e.g. MASCA, RASPLAV) to reactor case, are foreseen.

The developed and verified models will be further used for benchmarking and improvement of simplified models of various system codes such as ICARE/CATHARE, MELCOR, ASTEC or Russian severe accident code SOCRAT.

# Technical progress during the first year

### Task 1.: Development and Improvement of the Physico-Chemical Model for the U-Zr-O Melt Oxidation on the Base of New Crucible Tests

Subtask 1.1.: The existing model for U-Zr-O melt oxidation will be updated to the 2-d case corresponding to a more realistic geometry of molten pool in crucible and bundle tests. On this base, pre-test calculations for the planned new crucible tests on corium melt oxidation at the LAVA (FZK, Germany) will be carried out. As a result, a matrix for the test series will be prepared in cooperation with collaborators from CEA and FZK (Germany).

Subtask 1.3.: For consideration of molten corium physico-chemical interactions with reactor walls, a model for U-Zr-O melt interaction with stainless steel under non-equilibrium conditions with temperature gradient in the cooled walls, will be developed on the base of available experimental data and coupled with the melt oxidation model.

### Task 2.: Development and Improvement of the Unified Thermal Hydraulic Technique (CONV Code) for Simulation of Multiphase Processes in Complex Domains of Convectively Stirred Melt

Subtask 2.1.: Modernization of an existing code CONV: including into code of a new procedure for solving elliptical equations with boundary conditions of Neumann for the correction of pressure and new developed numerical scheme of the highest order of accuracy for solving of equations system of Navier-Stokes.

Subtask 2.3.: Conducting of numerical experiments for the choice of optimum turbulence model (algebraic type) using results of both convection in a cavity with the walls with different temperatures and convection of a heat-generating fluid, and model implementation in the CONV code.

# Technical progress during the year of reference

### Task 1.: Development and Improvement of the Physico-Chemical Model for the U-Zr-O Melt Oxidation on the Base of New Crucible Tests

Subtask 1.3.: For consideration of molten corium physico-chemical interactions with reactor walls, a model for U-Zr-O melt interaction with stainless steel under non-equilibrium conditions with temperature gradient in the cooled walls, will be developed on the base of available experimental data and coupled with the melt oxidation model.

* The model for oxidation of stainless steel was further developed by improvement of the numerical algorithms used for solution of the complicated problem of physico-chemical interactions between the molten corium and vessel walls, testing of the new algorithms against various temperature scenarios.
* Testing of the improved numerical algorithms revealed more reliable operation of the numerical scheme, quick convergence of calculations with respect to the time step and mesh size. Numerical calculation errors were evaluated, recommendations for practical choice of the numerical scheme parameters were elaborated.

### Task 2.: Development and Improvement of the Unified Thermal Hydraulic Technique (CONV Code) for Simulation of Multiphase Processes in Complex Domains of Convectively Stirred Melt

Subtask 2.4.: Improving of the turbulence model: coordination of algebraic model with large eddy simulation approach. Selection of a set commutative filters for a LES approach of a turbulence modeling and its implementation in CONV code. Adaptations of a code in view of requirements of the design LIVE facility.

* For improving of turbulence modeling at extremely high Rayleigh numbers LES approach was included in CONV code. The set of commutative filters for LES approach was chosen.
* The adaptation of CONV code for LIVE facility conditions is carried out by means of inclusion of model of the stratified convection with the purpose of modeling and estimation of a focusing effect. Testing the modernized version of CONV code was continued on such tests as: Backward-facing step flow, T-junction thermal mixing test and also series of experiments on LIVE facility. In all cases the good agreement was obtained. The results were published in journal Progress in Nuclear Energy 52 (2010) 46-60 (M. Buck, M. Buerger, A. Miassoedov, X. Gaus-Liu, A. Palagin, L. Godin-Jacqmin, C.T.Tran, W.M. Mad, V. Chudanov, The LIVE program -Results of test L1 and joint analyses on transient molten pool thermal hydraulics).
* The parallel version of the CONV code in MPI standard was developed for the carried out calculations of the cluster machines with < =256 processors.

### Task 3.: Tight Coupling of the Two Advanced Tools: the Physico-Chemical (Molten Pool Oxidation) Model and the Thermo-Hydraulic Code CONV, for Realistic Mechanistic Description of U-Zr-O Molten Pool Behaviour in Oxidising Test Conditions

Subtask 3.1.: The modified melt oxidation model will be upgraded to the geometry of molten pool confined by the walls of reactor pressure vessel. An interface of the melt oxidation numerical module for coupling with the thermal hydraulic code CONV will be elaborated.

* The melt oxidation model that simulates evolution of the solid phase layers ((Zr,U)O2-x crust, FeO corrosion layer and steel), temperature distributions in the layers and U, Zr, O molar fluxes into the melt, was modified and upgraded to the geometry of molten pool confined by the walls of reactor pressure vessel.
* An interface of the melt oxidation numerical module for coupling with the thermal hydraulic code CONV was elaborated.

Subtask 3.2.:Preparatory work with the code sources for implementation of melt oxidation model, and also interface (input files) for insert of physicochemical melt oxidation model for modeling of thermal hydraulic behavior of U-Zr-O melt under oxidizing for small and medium scale experiments in the code CONV 2D.

* Preparatory work with the code sources for implementation of melt oxidation model is carried out.
* The interface (input files) for insert of physicochemical melt oxidation model for modeling of thermal hydraulic behavior of U-Zr-O melt under oxidizing for small and medium scale experiments in the code CONV 2D is prepared. The given set includes an additional orthogonal grid, on which the quasi one-dimensional melt oxidation model will be solved. The grid will be connected on boundary conditions with a base calculated grid of the CONV code. Besides the parameter set includes characteristics of materials, participating during oxidation, which with the help of the interface program will be transformed to a set of entering files for the CONV code, taking into account chemical structure (component and amount moles), property (thermal capacity, thermal conduction, denseness, viscosity), temperature cooperating steel and melt for an interchanging with melt oxidation model.
* Testing the modernized version of the CONV code is continued on such tests as T-junction thermal mixing test usage of parallel version of the CONV code. A good agreement for the finest grids up to 40 millions nodes is obtained.

# Current technical status

1. on schedule

# Cooperation with foreign collaborators

* Signing of the additional Agreement with the Project collaborator FZK (Germany) on information exchange and delivery to FZK of the SFPR code, developed at IBRAE partially within the current and previous (#2936) ISTC Projects.
* Delivery to the Project collaborator FZK (Germany) of the upgraded version of the computer code SVECHA, developed at IBRAE within bilateral Agreement with FZK, for analysis of ongoing at FZK separate-effect tests.

#### Preparation of the Report on recommendations and critical analysis of the experimental results of the ISTC Project METCOR used in the current Project for the development of the model on corium melt interactions with vessel steel «Critical comments to results of the METCOR tests and to their interpretation» and discussion it with the Project Collaborators.

* Participation in the 15th International QUENCH Workshop, organized by the Project collaborator FZK (Germany) with presentation of the main results of the ISTC Project #3876 by the Project manager, November 2009.
* Participation in the 13th International Topical Meeting on Nuclear Reactor Thermal Hydraulics (NURETH-13), September 27 - October 2, 2009. Kanazawa, Japan.
* Participation in the 17th Meeting of the Contact Expert Group on Severe Accident Management (CEG-SAM) in CIEMAT, Madrid, March 29-31, 2010.
* Participation in the 18th Meeting of the Contact Expert Group on Severe Accident Management (CEG-SAM) in NITI, St.-Petersburg, September 28-30, 2010.

# Perspectives of future developments of the research/technology developed

In accordance with the Project Working Plan.

**Attachment 1:** List of papers and reports with abstracts published during the year of reference

**1. Joint publication with Project collaborators in: Progress in Nuclear Energy 52 (2010) 46–60.**

**M. Buck, M. Buerger, A. Miassoedov, X. Gaus-Liu, A. Palagin, L. Godin-Jacqmin, C.T.Tran, W.M. Mad, V. Chudanov, “The LIVE program –Results of test L1 and joint analyses on transient molten pool thermal hydraulics”.**

**Abstract**

The development of a corium pool in the lower head and its behaviour is still a critical issue. This concerns, in general, the understanding of a severe accident with core melting, its course, major critical phases and timing, and the influence of these processes on the accident progression as well as, in particular, the evaluation of in-vessel melt retention by external vessel flooding as an accident mitigation strategy. Previous studies were especially related to the in-vessel retention question and often just concentrated on the quasi-steady state behaviour of a large molten pool in the lower head, considered as a bounding configuration. However, non-feasibility of the in-vessel retention concept for high power density reactors and uncertainties e.g. due to layering effects even for low or medium power reactors, turns this to be insufficient. Rather, it is essential to consider the whole evolution of the accident, including e.g. formation and growth of the in-core melt pool, characteristics of corium arrival in the lower head, and molten pool behaviour after the debris re-melting. These phenomena have a strong impact on a potential termination of a severe accident. The general objective of the LIVE program at FZK is to study these phenomena resulting from core melting experimentally in large-scale 3D geometry and in supporting separate-effects tests, with emphasis on the transient behaviour.

Up to now, several tests on molten pool behaviour have been performed within the LIVE experimental program with water and with non-eutectic melts (KNO3-NaNO3) as simulant fluids. The results of these experiments performed in nearly adiabatic and in isothermal conditions, allow a direct comparison with findings obtained earlier in other experimental programs (SIMECO, ACOPO, BALI, etc.) and will be used for the assessment of the correlations derived for the molten pool behaviour. Complementary to other international programs with real corium melts, the results of the LIVE activities also provide data for a better understanding of in-core corium pool behaviour.

The experimental results are being used for the development and validation of mechanistic models for the description of molten pool behaviour. In the present paper, a range of different models is used for post-test calculations and comparative analyses. This includes simplified, but fast running models implemented in the severe accident codes ASTEC and ATHLET-CD. Further, a computational tool developed at KTH (PECM model implemented in Fluent) is applied. These calculations are complemented by analyses with the CFD code CONV (thermal hydraulics of heterogeneous, viscous and heat-generating melts) which was developed at IBRAE (Nuclear Safety Institute of Russian Academy) within the RASPLAV project and was further improved within the ISTC 2936 Project.

**2. V.V. Chudanov, A.E. Aksenova, V.A. Pervichko, A.A. Makarevich, N.A. Pribaturin, O.N. Kashinskii.** **3D CFD CONV CODE: VALIDATION AND VERIFICATION in Proceedings CFD for Nuclear Reactor Safety Applications CFD4NRS3 Workshop, September 14-16, Bethesda North Marriott Hotel & Conference Center. 2010.**

**Abstract**

During some years in IBRAE a set of 3D CFD modules (CONV code) for safety analysis of the operated Nuclear Power Plants (NPPs) is developing. These modules are based on the developed algorithms with small scheme diffusion, for which the discrete approximations are constructed with use of finite-volume methods and fully staggered grids. The CONV code is fully parallelized and highly effective on high performance computers. The developed modules were validated on a series of well known tests in a wide range of Rayleigh numbers (106-1016) and Reynolds numbers (103-105). In this paper the examples of use of the developed software for modeling a fuel assembly, namely, for researching a hydraulic resistance factor of a spacer, are demonstrated. The calculations are carried out on a sequence of condensed grids with an amount of nodes from a range 107-108, for which the convergence was obtained. Moreover, the attention of this paper is focused on validation and verification of the software with usage of such tests as: 3D convection in a lid-driven cavity flow, turbulent flow of water in a round pipe, backward-facing step flow and T-junction thermal mixing test. In all cases a good agreement was obtained.

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| **Attachment 2:** | List of presentations at conferences and meetings with abstracts |

### Modelling of U-Zr-O corium/ vessel steel interactions (ISTC Project #3876)

M. Veshchunov, IBRAE

### Presented at the 15th International QUENCH Workshop in FZK (Germany), November 2010.

**Abstract**

Current results of the ISTC project #3876 THOMAS are presented. The main stages of molten U-Zr-O corium interactions with vessel steel (VS) walls are analysed. During the initial transient stage a rapid ablation of VS takes place under formation of a solid or mushy (depending on oxygen content in the melt) crust controlled by rapid heat exchange processes accompanied with mixing of the melt. This stage can be generally described by thermo-hydraulic codes.

During the subsequent steady state stage the heat and mass exchange processes between melt, crust and walls should be considered self-consistently, taking into account steep temperature gradients and oxidizing conditions in the melt. During this stage, the following physico-chemical processes simultaneously take place: conversion of the crust from a mushy to solid one, accompanied with a growth of the formed crust, and corrosion (oxidation) of the VS walls, which are strictly controlled by oxygen transport through the multilayered structure. The growth of the solid crust due to oxygen transport through the melt to cold walls is described by the SVECHA Melt Oxidation (MO) model, developed within the previous ISTC Project #2936, which will be refined on the basis of new FZK crucible tests within the current project.

The corrosion of VS walls is analyzed using the experimental data from the ISTC Project METCOR. The available SVECHA model for steel oxidation in steam and which is based on the parabolic correlation derived from the KI tests for 06Х18Н10Т steel is modified for 15 Kh2NMFA vessel steel (using METCOR data) and supplied with the “oxygen starvation” regime consideration, in which VS oxidation kinetics is controlled by external oxygen flux. The starvation regime is valid during relatively long period of corrosion when the corrosion layer is relatively thin in comparison with the crust thickness, thus, transport of Fe and/or oxygen ions through this layer is a relatively quick process and its growth is controlled by the oxygen flux from the (solid or mushy) crust.

The VS corrosion model is numerically realized and implemented in the melt oxidation (MO) model. The new model was tested and then applied to typical temperature scenarios of tests carried out in the on-going ISTC project METCOR-P.

The model allows interpretation of the main test observations and qualitatively describes VS corrosion kinetics observed in low- and high-temperature regimes. The interactions become especially complicated in high temperature tests with eutectic formation at the interface between corrosion (FeO) and crust (U,Zr)O2 layers. This results in accelerated VS corrosion kinetics described by the new model using “flowering” mechanism. After additional refinement and validation, it is foreseen to start modification of the new physico-chemical interactions model and its preparation for implementation in the thermal-hydraulic code CONV.

1. **Status 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)**

Presented by M.S. Veshchunov and V.V. Chudanov at the 17th CEG-SAM in CIEMAT, Madrid, March 29-31, 2010.

**Abstract**

The progress report on the ISTC Project #3876 (THOMAS) obtained during 5-6 Quarters is presented.

**Part 1.** 1-D numerical model for U-Zr-O corium melt – steel oxidation and its implementation into the 2-D thermo-hydraulic code.

A preparatory work for implementation of the physico-chemical interactions model, developed in the previous stage of the Project, in the thermo-hydraulic code CONV was carried out.

The 2-D stand-alone code developed to simulate (in the simplified geometry of the tests) simultaneous UO2 fuel dissolution, U-Zr-O corium melt oxidation accompanied with the bulk ceramic precipitates formation and oxidation of the steel wall of a vessel in contact with corium, was transformed into the 1-D corium melt – steel oxidation module, in order to describe local interactions at the corium-steel interface (in the geometry of the pressure vessel). This allows to exclude from the code a simplified description of the heat and mass exchange between the U-Zr-O corium melt and peripheral crusts, and to use (in future) detailed thermo-hydraulic approach of the CONV code.

The resulting new 1-D oxidation numerical module simulates evolution of the solid phase layers ((Zr,U)O2-x crust, FeO corrosion layer and steel), temperature distributions in the layers and U, Zr, O molar fluxes into the melt. Two types of multilayer structure geometry is considered – cylindrical and plane.

1-D oxygen mass transfer in the (Zr,U)O2-x crust is simulated by numerical solution of the partial derivative diffusion equation with moving boundaries. The oxygen boundary concentrations are determined using the equilibrium Zr-O phase diagram. Relocation of the boundary between the corium melt and solid ceramic crust is calculated by matching the oxygen fluxes in the melt and ceramic crust at the interface.

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 weight gain is controlled by the oxygen flux from the crust. For high temperatures above the FeO – ZrO2 eutectic point, the new model (developed in the previous stage of the Project) simulating an enhanced (in fact, instantaneous) extrusion of the eutectic melt into the corium through the crust, is realized.

Temperatures of the solid multilayer structure are calculated using linear spatial profile approximation (in the thin wall layers geometry) taking into account heat effects of oxidation.

Evolution of U-Zr-O corium melt temperature and composition distributions is calculated by the 2-D thermo-hydraulic code CONV. The oxidation module is coupled with the 2-D thermo-hydraulic code through the heat and oxygen mass fluxes from the melt to 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 1-D oxidation module. Oxidation module is called for each thermo-hydraulic spatial mesh at the melt-solid interface.

The interface program unit for coupling of the melt – steel oxidation 1-D module with the corium melt 2-D thermo-hydraulic code is developed. 1-D oxidation module is currently under implementation into the 2-D thermo-hydraulic code and will be completed during 7-8th Quarters.

**Part 2.** Development and improvement of the unified thermal hydraulic technique (CONV code) for simulation of multiphase processes in complex domains of convectively stirred melt.

For improving of turbulence modeling at extremely high Rayleigh numbers, LES approach was included in CONV code. The modeling of a large-scale turbulence is based on a turbulence filtration and in essence this method is more universal, since the immediate restriction on magnitude of Reynolds number does not superimpose. The results of choice set of commutative filters for LES approach are presented.

Results of verification of the modified version of CONV code against Backward-facing step flow tests and T-junction thermal mixing tests are discussed.

The method of a large-scale turbulence modeling is applied to testing semi-empirical models.

1. **Progress Report on the ISTC project #3876 “Thermo-hydraulics of U-Zr-O molten pool under oxidising conditions in multi-scale approach (crucible - bundle - reactor scales)” (THOMAS).**

Presented by M.S. Veshchunov and V.V. Chudanov at the 18th CEG-SAM in NITI, St.-Petersburg, September 28-30, 2010.

**Abstract**

The progress report on the ISTC Project #3876 (THOMAS) obtained during 7-8 Quarters is presented.

The 2-D stand-alone code developed to simulate (in the simplified geometry of the tests) simultaneous UO2 fuel dissolution, U-Zr-O corium melt oxidation accompanied with the bulk ceramic precipitates formation and oxidation of the steel wall of a vessel in contact with corium, was transformed in the previous stage of the Project (Quarters 5-6) into the 1-D corium melt – steel oxidation module, in order to describe local interactions at the corium-steel interface (in the geometry of the pressure vessel). This allowed to exclude from the code a simplified description of the heat and mass exchange between the U-Zr-O corium melt and peripheral crusts, and to use (in future) detailed thermo-hydraulic approach of the CONV code.

The work for further development and testing against experimental data of the 1-D oxidation numerical module that simulates evolution of the solid phase layers ((Zr,U)O2-x crust, FeO corrosion layer and steel), temperature distributions in the layers and U, Zr, O molar fluxes into the melt, was continued. Further improvement of interface program unit for coupling of the melt – steel oxidation 1-D module with the corium melt 2-D thermo-hydraulic code was continued.

Preparatory work with the code CONV 2D sources for implementation of melt oxidation model, and also interface (input files) for insert of physicochemical melt oxidation model for modeling of thermal hydraulic behavior of U-Zr-O melt under oxidizing conditions for small and medium scale experiments in code CONV 2D was continued.

Designing the interface program unit for the representation of a minimum parameter set for melt – steel oxidation 1-D module was continued. The given set includes an additional orthogonal grid, on which the quasi one-dimensional melt oxidation model will be solved. The grid will be connected by the boundary conditions with a base calculated grid of CONV code. Besides the parameter set includes characteristics of materials, participating during oxidation, which with the help of the interface program will be transformed to a set of entering files for CONV code, taking into account the chemical structure (molar composition), property (thermal capacity, thermal conduction, denseness, viscosity), temperature cooperating steel and melt for an interchanging with melt oxidation model.

Testing the modernized (parallel) version of CONV code was continued on such tests as T-junction thermal mixing test. A good agreement for the finest grids up to 40 millions nodes was obtained.

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| **Attachment 3:** | Illustrations attached to the main text |

**METCOR Tests, their Interpretation & Application to Modelling of Corrosion & Diffusion.**

This Memo resulted from an attempt to model the results of the METCOR tests with the new model under development in the THOMAS Project. This proved to be difficult and on reviewing M. Veshchunov (IBRAE) came up with several inconsistencies in the METCOR test results and the models proposed. D. Bottomley (ITU), the associate of the METCOR Project, evaluated these comments and reduced this to a list of valid criticisms, followed by a short proposal (the additional document) on how the conflict between the modelling & experimental results can be resolved with an appropriate experiment or modelling effort/development.

1. Normally tests on the kinetics of various physico-chemical interactions are performed using one test (at fixed temperature) for each time point + detailed post-test measurements of the main characteristics (interaction layers thickness, their chemical composition, oxygen profiles, etc.), cf. crucible tests of FZK (KfK), IRSN, CEA, etc. Only on this basis consistent interpretation and mechanistic modeling of the test results can be attained. In the subsequent stages of the research, more complicated tests in more prototypic conditions can be used for verification of the developed models.

The obtained results of METCOR tests [1-4], having rather complicated temperature scenarios (that are prototypical of the reactor conditions), are essentially based on on-line measurements and for this reason, as will be shown below, in many cases become rather uncertain and their interpretations – mutually contradictory. Most reliable data were obtained from post-test measurements; however, since the tests scenarios were rather complicated (several temperature plateaus), only qualitative information can be deduced with confidence from these data. This essentially complicates mechanistic modeling of the corrosion effect.

2. The measured kinetic data are presented in the simplest form of Tamman’s equation that is valid for a *single* interaction layer. However, this equation is applied in METCOR to consideration of *two-layer* system (i.e. corrosion layer + corium crust); this requires an additional assumption on the rate-determining process (or layer), that is often rather inconsistent in the METCOR analysis:

Indeed, in the tests with UO2+x-ZrO2-FeOy corium (MC-2, MC-3) the measured data are described under assumption that “*the crust layer does not provide any resistance to Fe diffusion*” and for this reason only the corrosion layer FeO is taken into consideration [2].

However, in [3] the same experimental data (for MC-2 test) are described under an exactly opposite assumption that “*main diffusion resistance for Fe2+ ions is the corium crust*” [4]. The tests with UO2+x-ZrO2 corium (MCP-2 and MC-10) are treated in a similar way disregarding the corrosion layer thickness. Nevertheless, the MC-3 test is still described in [3] excluding the crust thickness from consideration, despite the experimental data show that, similarly to MC-2 test, the crust thickness (3-10 mm, see Figs. 18 and 24 from [1]) is notably thicker than the corrosion layer (< 1 mm).

It may be really difficult to decide which the rate-determining layer is. In order to avoid this uncertainty, the general diffusion theory for the physico-chemical interactions recommends considering diffusion through the *two-layer* system (crust + oxide), as attempted (following this theory) in the THOMAS model. Naturally this approach is much more complicated, since it requires self-consistent consideration of diffusion transport in different interaction layers, flux matches at their interfaces and mass balances in the system. For this reason, more precise and detailed experimental data are required for such an approach.

3. Additionally it is assumed in METCOR that the governing process in corrosion kinetics is iron (Fe2+) diffusion through the layers. This assumption is definitely correct (as known from the literature) for the corrosion (FeO) layer growth in oxidizing atmosphere (under unlimited oxygen supply), however, it might be mistaken for the corrosion layer growth under limitation on oxygen supply induced by the adjacent (rather thick) crust layer, and questionable in application to the crust layer (at least, in the case of the (U,Zr)O2 crust).

Besides, a notable dependence of the corrosion rate on the oxygen potential in the melt revealed in the tests can be hardly explained and described neglecting consideration of oxygen diffusion in the interaction system. Indeed, in accordance with [4]: “*Drop in the oxygen potential of the melt is detected when heated steel has a high oxidation rate; Lower corrosion rate at the final stage of experiment is explained by the insufficient air supply to the melt and by its decreased oxygen potential*”.

These observations give an important confirmation that a theoretical model cannot avoid consideration of oxygen transport through the interaction layers, which, of course, should be self-consistently combined with consideration of Fe ions diffusion through the oxide (corrosion) layer (as attempted in the THOMAS model).

4. Another confirmation of this statement concerning key importance of the oxygen transport through the reaction layers (ignored in the METCOR model), can be deduced from the “high-temperature” tests with eutectic liquid layer formation at the interface with the steel.

Indeed, in the last phases of MCP-2 (*TS* > 1300°C) “*the corrosion layer contained a completely or mainly liquid phase which was determined by the SEM/EDX analysis*” with an extremely small thickness (≈ 200μm) in comparison with the corrosion depth (≈ 5 mm). This observation was also explained in METCOR by Fe diffusion through the crust (with a thickness of several mm): “*The mass flow of Fe2+ ions from the steel surface through corrosion layer is accompanied by the mass transfer of Fe2+ ions from the surface of corrosion layer through the corium crust into the melt, and with the counter-flow of oxygen ions*” [3], see Fig. 1.



Fig. 1. Schematics of diffusion processes in the steel-adjacent layers (from [3]).

Being focused on consideration of Fe ions diffusion transport through the crust to the corium melt, the METCOR analysis completely ignores the problem concerning the oxygen balance in the corrosion FeO layer. Indeed, as explained in [1], under lower temperatures (*TS* < 1300°C) when liquefaction of FeO did not take place, its thickness roughly corresponded to the corrosion depth (see below Fig. 2 taken from [1]). In the considered case of high *TS* in the last stage of MCP-2 (when FeO phase was completely liquefied owing to eutectic interactions with the crust), within the corrosion depth (of ≈ 5 mm) only a very thin corrosion layer (of ≤ 200 μm) was retained in-between steel and the crust (see post-test Fig. 3 taken from [3]), despite a thick FeO layer of several mm (!) was formed during the previous stages of interactions. This implies that not only Fe, but also O atoms had to release through the crust in the late (“eutectic”) stage of corrosion (that cannot not be explained by the oxygen diffusion, especially under METCOR assumption that oxygen ions continue to counter-flow from the melt through the corium crust into the surface of corrosion layer*,* as shown in Fig. 1).

This was the main reason why a new (“flowering”) mechanism was proposed in the THOMAS Project, that allowed consistent explanation of strong reduction of the reaction layer thickness (from ≈ 5 to mm ≤ 200 μm) by extrusion of the eutectic melt (containing both Fe and O !) through the crust into the corium, resulting in remarkable acceleration of the corrosion kinetics. In the literature a qualitatively similar “drainage” mechanism was discussed (see below).

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| Fig. 2. 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, (5) crust (from [1]) | Fig. 3. Microstructure of interface between steel (lower, grey layer) and (U,Zr)O2 crust (upper, white layer) in MCP-2 test (from [3]). |

4.1. In the subsequent critical analysis [4] of the flowering mechanism, it was claimed that “*The flat steel surface in METCOR does not produce a compressing impact on the FeO layer (differently from a cylindrical fuel rod). There are no reasons for stochastic (in time and space) generation of cracks in the crust (flowering)*”. To confirm this statement, it was argued that in a more simple geometry of METCOR tests the crust could freely relocate upward coherently with expansion of underlying layer (owing to transformation Fe→FeO).

As explained in the THOMAS presentation (referred to in [4]), “At high temperatures eutectic melt is extruded through the tears/cracks into the corium (owing to high compressive stresses in eutectic melt)”. It was also commented there that the first possibility (tears at the periphery of crust at the contact line with the walls, leading to “floating” of the crust) seems to be the most probable mechanism (however, cracks are also possible). In other word, as soon as the crust start to relocate upward (i.e. to float), the eutectic melt (being under high pressure) is extruded through the formed tear between crust and walls into the corium.

Such a conclusion was derived mainly from the theoretical consideration. Nevertheless, some experimental observations of large cracks in [3] cannot be ignored as well: “The presence of tree-like branching cracks typical of the stress corrosion cracking regime is observed closer to the central part”, see Fig. 3.

4.2. Another critical comment of [4]: “*Even if the generation of cracks takes place, they are healed during the corium melt ingress by low local temperatures [see the dissertation of Yu. Petrov]*”, does not really contradict to the THOMAS presentation: “At low temperatures (no FeO-crust eutectics formation) corium melt penetrates into tears/cracks, immediately freezes and thus heals them over”. However, at higher temperatures the eutectic melt penetrating under high pressure through the cracks (or tears) will apparently not freeze.

5. In evaluation of the crust + corrosion layer thickness  , that is the key parameter in the proposed METCOR correlation for the corrosion rate, it is assumed that “ *is temperature of corium crust adjacent to the melt, which is equal to solidus temperature of crust average composition”* (further evaluated as the eutectic temperature for the corium, i.e. ≈ 2450°C for UO2+x-ZrO2 corium and 1340°C for UO2+x-ZrO2-FeOy corium).

In reality it easy to see, for example from consideration of the simplest cases of pure ZrO2 or UO2 oxides, Fig. 4, that  is a strong function of *oxygen content at the interface of the crust* with the melt, and thus can vary *within several hundreds K* depending on temperature in the bulk of melt and the heat flux  from melt to walls. So, even in these simple cases  cannot be fixed as a predetermined value (e.g. ≈ 2450°C), i.e. it should be calculated from mass and heat balances and flux matches at the interface (as attempted in the THOMAS model).

Solidus line

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Fig. 4. Equilibrium Zr-O and U-O phase diagrams from THERMODATA [P.-Y. Chevalier, E.Fischer, B. Cheynet, “Progress in the thermodynamic modelling of the O–U–Zr ternary system”, Computer Coupling of Phase Diagrams and Thermochemistry 28 (2004) 15–40]

A similar strong variation of the solidus temperature can be also demonstrated for the mixed (U,Zr)O2 oxides (that can be readily deduced from the available ternary U-Zr-O phase diagrams, Fig. 5).

solidus

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Fig. 5. Equilibrium ternary U-Zr-O phase diagrams from THERMODATA [P.-Y. Chevalier, E.Fischer, B. Cheynet, “Progress in the thermodynamic modelling of the O–U–Zr ternary system”, Computer Coupling of Phase Diagrams and Thermochemistry 28 (2004) 15–40]

This conclusion (concerning erroneous evaluation of the solidus temperature) can be confirmed by direct comparison of the measured and calculated values of  (corrosion layer + crust thickness), using the METCOR expression . Indeed, for instance for phase 3 of MC-3 test, using available in [3] data for the parameters of this expression (≈ 1100°C, ≈ 0.33 MW/m2, ≈ 2-4 W/m⋅K, *Tsol*≈ 1340°C), it is straightforward to estimate ≈ 1-3 mm, whereas measurements of the crust thickness  (which is only a part of ) give one order of magnitude larger value ≈ 10 mm, see Fig. 5 (red circles).

This is a serious inconsistency of the main correlation for the corrosion rate, derived in the METCOR Project.



Fig. 6. Experimental data for MC-3 test (fig. 18 from [1]).

6. “*In accordance with the THOMAS model, a transition from “low” to “high” temperatures should always result in the qualitative changes of corrosion process. But this is not observed in case of UO2+x-ZrO2 corium*” [4].

This is really very important statement of the THOMAS model that is in apparent contradiction with the METCOR test data (or their interpretation). Analysis of *post-test* METCOR data (based on microstructure observations from Fig. 3 along with the measurement of a rather thick final corrosion depth ≈ 5 mm (!) in MCP-2 test) allowed making such a conclusion. As explained above, this discrepancy can be apparently associated with the on-line measurements.

Moreover, it should be noted that a similar effect of rapid eutectic penetration in vessel steel interacting with hot ceramic material (crust) was described the literature (in 80-90-ies). For instance, in SA research Review paper for Fast Breeder Reactors [5], the rapid eutectic penetration temperature of the steel was lowered to approximately 1400 K.

A similar effect of steel corrosion acceleration, owing to steel liquefaction on the interface between the steel wrapper and U-Zr-O corium crust and “drainage” of the formed melt into corium, was studied, e.g., in the SCARABEE tests [6].

Despite these integral tests were too complicated to get information on the kinetics, they clearly revealed an important qualitative result on abrupt acceleration of the corrosion rate above a certain temperature threshold. Contrary to the integral tests, the METCOR tests give a unique opportunity to measure the corrosion kinetics in well-defined conditions, if simple temperature scenarios (with one temperature plateau) will be used. Results of these tests will allow re-examination of the previous test data and resolving the numerous (above described) inconsistencies in their interpretation. Besides, these results will provide the necessary test matrix for verification of the THOMAS or other mechanistic models, that are requested for development of the best-estimate SA codes (free from semi-empirical, parametric models and correlations).

For this reason, corresponding modification of scenarios of new (planned) METCOR tests, supplemented with detailed post-test examinations, is strongly recommended.

References

1. S.V. Bechta et al., “Corrosion of vessel steel during its interaction with molten corium. Part 1: Experimental”. Nuclear Engineering and Design 236 (2006) 1810–1829
2. S.V. Bechta et al., “Corrosion of vessel steel during its interaction with molten corium. Part 2: Model development”. Nuclear Engineering and Design 236 (2006) 1362–1370
3. S.V. Bechta et al., “VVER vessel steel corrosion at interaction with molten corium in oxidizing atmosphere”. Nuclear Engineering and Design 239 (2009) 1103–1112
4. Progress Report on the ISTC project #3592 “Investigation of Corium Melt Interaction with NPP Reactor Vessel Steel (METCOR-P) ”. Presented by S. Bechta at the 17th CEG-SAM meeting, Madrid, Spain, March 29-31, 2010
5. “Severe Accident Approach – Final Report Evaluation of Design Measures for Severe Accident Prevention and Consequence Mitigation”. Prepared by A.M. Tentner, ANL-GENIV-128, March 2010.
6. G. Kayser, R. Stansfeld, “SCARABEE experimental expertise on failure mechanisms of stainless steel walls attacked by molten corium”. Proc. Advanced Reactor Safety Meeting, Pittsburg, PA, 1994.