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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, 2008 to September 30, 2009 | | |
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| Director | Leonid A. Bolshov  Dr., Professor | 30.09.09 |

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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: |  |
| Commencement Date: | October 1, 2008 |
| Duration: | 3 years |
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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 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 1.1.: 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).

* + The physical model and 2-d numerical module are developed for analysis of the crucible tests on corium melt oxidation. This model was used for pre-test calculations of the crucible tests planned at the LAVA facility (FZK, Germany).
  + The models for the mushy zone evolution and stainless steel (SS) oxidation are developed for analysis of the corium melt oxidation and interactions with SS walls.

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 implemented in the general model corium oxidation and physico-chemical interaction with walls.
* The model for oxidation of stainless steel was extended to consideration of eutectic interactions of SS oxide with corium crust at relatively high temperatures and implemented in the general model corium oxidation and physico-chemical interaction with walls.
* Comparison of the calculation results on the crust formation on the interface between corium and cooled walls and corrosion effect of corium on the stainless steel walls under high heat flux conditions with results of the METCOR experiments demonstrated qualitative agreement of the model predictions with observations.

### 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.

* The code CONV was modernized by including a new procedure for solving elliptical equations for the correction of pressure and new developed numerical scheme of the highest order of accuracy for solving of Navier-Stokes equations.
* The new procedure for solving elliptical equations with boundary conditions of Neumann for the correction of pressureis based on the modified Richardson iterative method with strongly variable factors using Fast Fourier Transformation algorithm as a preconditioner.
* The developed numerical scheme for solving of Navier-Stokes equations is based on a principle of splitting on physical processes. For solving of a convective part of Navier-Stokes equations the new effective scheme for solving of advection equations of higher order and with both low amplitude and dispersing errors is proposed.
* Thus new possibilities were obtained: calculations on non-uniform grids and at different types of boundary conditions.

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.

* The numerical experiments at the choice of optimum turbulence model (algebraic type) are carried out. Among them are 1) approximated turbulence model, 2) algebraic turbulence model (Bolduin-Lomax) and 3) quasi DNS (QDNS) approach.
* The code CONV was modernized by including approximated turbulence model and QDNS approach.
* The modified CONV code was validated on such tests, as: convection in a cavity with the walls with different temperatures and convection of a heat-generating fluid. For all cases a good agreement of numerical predictions with experiment was obtained.

# Current technical status

1. on schedule

# Cooperation with foreign collaborators

1. Cooperation Agreement between IBRAE and FZK (Project Collaborator) on the exchange of experimental data and numerical programs developed within the ISTC Project, was signed
2. IBRAE transfers to Forschungszentrum Karlsruhe (FZK) the CONV2D/3D code developed in the framework of the ISTC Project #2936 and improvements and updates of this code which will be performed in the framework of the ISTC Project #3876 and provides support to Forschungszentrum code users
3. Preparation of joint publications with FZK collaborator Discussion and preparation of the test matrix for the experiments to be carried out at the LAVA facility (FZK)
4. Organization of the international scientific and technical meeting «Computational and experimental studies of LWR fuel element behavior under beyond design basis accidents and reflood conditions», has been carried out in July 27-28 at IBRAE (Moscow)
5. Participation in the 14th CEG-SAM Meeting (Kiev, September 2008);

Participation in the 15th CEG-SAM Meeting (Villigen, March 2009);

Participation in the 16th CEG-SAM Meeting (Moscow, September 2009).

# 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. J. Stuckert, M. S. Veshchunov, “Behaviour of the cladding oxide layer under steam starvation conditions”. FZKA 7373, Forschungszentrum Karlsruhe, April  
   2008.

**Abstract**

Results of the tests on the long duration annealing of pre-oxidized Zircaloy cladding tubes in the inert atmosphere with the annealing temperatures between 1250 and 1500 °C and a corresponding model are presented. The objective of the tests was the investigation of the reduction kinetic of the oxide layer during the steam starvation phase by the progression of core drying during the severe accident. The homogeneous formation of the α-Zr(O) precipitations inside of the oxide layer and formation of the α-Zr(O) scale on the cladding outer surface were detected in addition to the oxide layer thickness change. The phenomenon should have a strong influence on the intensive hydrogen release during the following quench phase.

1. M.S. Veshchunov, “Modelling of a Thin Mushy Layer Evolution during Binary Solid-Liquid Interactions”, Journal of Engineering Thermophysics, vol. 18, № 2, 2009

**Abstract**

Further development of the Brody-Flemings approximation in application to a thin mushy zone at the interface between binary liquid and solid phases, typical in the context of corium evolution in the reactor pressure vessel during severe accidents at Nuclear Power Plants, is presented. The main assumption of the Brody-Flemings approximation concerning local equilibrium between the solid and liquid phases in the two-phase zone is confirmed for the considered case of a thin mushy layer and supplemented with the heat and diffusion flux matches at its interfaces. This approach allows a relatively simple description of the mass and heat transfer through the mushy zone along with the zone formation, growth and/or shrinkage (depending on varying external conditions) in the course of solid-liquid material interactions. In order to prove consistency of the developed approach, two important limiting cases, when the solidification rate is controlled either by the diffusion of heat or by solute diffusion, are studied analytically in the steady-state approximation. It is shown that in both limiting cases explicit expressions for the mushy zone thickness are directly associated with the criterion of the plane front instability. In particular, this implies that the emergence or vanishing of the mushy zone in the course of liquid-solid interactions is described in a self-consistent manner in the developed approach.

1. V. Chudanov, A.Palagin and F.Kretzschmar, LIVE test FSt4: experimental results and simulation by CONV code, Proc. 13th International Topical Meeting  
   on Nuclear Reactor Thermal Hydraulics (NURETH-13), September 27 - October 2, 2009. Kanazawa, Japan, Paper N13P1076, CD-ROM.

**Abstract**

3-D thermohydraulic CFD code CONV was applied to the simulation of FSt4 LIVE water test. Two calculations were performed: in the first one the homogeneous heating of liquid was assumed, in the second one the spiral heaters actually used in the test were modelled. The results of these two calculations were compared with each other and with the experimental data. The obtained results shows that there is no critical difference in the heat flux distribution at the vessel wall for these two cases, indicating that the LIVE facility adequately represents thermal conditions of the homogeneously heated liquid.

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

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)**

Представлено М.С. Вещуновым на заседании 14th CEG-SAM (Киев, сентябрь 2008)

Presented by M.S. Veshchunov (IBRAE)

Status and general information on the Project THOMAS recently approved by ISTC Governing Board for funding (GB#46), will be presented. This includes information on leading Institution IBRAE, Moscow), foreign collaborators (FZK, IRSN, CEA, ITU, IVS Trnava), duration (3 years), total cost (Euro 196 850), organizational structure, technical approach and methodology, interconnection with other projects, time schedule and main objectives.

Expected and preliminary results of the Project will be outlined.

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)**

Представлено на заседании 15th CEG-SAM (Виллиген, март 2009 г.)

Presented by M.S. Veshchunov and V.V. Chudanov (IBRAE)

The current status of the Project THOMAS is presented. This includes brief general information on the Project organization, main objectives and time schedule. In more details results of Tasks 1 and 2 obtained during 1-2 Quarters are outlined.

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

Main stages of molten U-Zr-O corium interactions with SS walls are analysed:

During initial transient stage rapid ablation of SS and formation of solid, or mushy (depending on oxygen content in the melt), crust controlled by (rapid) heat exchange processes accompanied with mixing of melt, in neglect of (slow) diffusional redistribution of components, take place. This stage can be generally described by thermohydraulic codes (e.g., to be realized in the CONV code).

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 gradient and oxidizing conditions in the melt. During this stage, the following physico-chemical processes simultaneously take place:

* Conversion from mushy to solid crust, accompanied with
* Crust growth,
* Corrosion (oxidation) of SS walls,

which are strictly controlled by oxygen transport through the multilayered structure.

Growth of the solid crust owing 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 base of new FZK crucible tests within the current Project.

Conversion (to solid) and growth of the mushy crust in steep temperature gradient is examined with the new analytical model (prepared and accepted for publication) based on the Flemings-Brody approach, which will be numerically realized in the subsequent stages of the Project. Solution of the heat- and mass-transfer equations with flux matches at the mushy-zone interfaces describes emergence of the two-phase zone precisely under Mullins-Sekerka condition for the plane front instability, this reflects self-consistency of the new model.

Corrosion of SS walls is analyzed using experimental data from the ISTC Project METCOR. The available SVECHA model for stainless steel oxidation in steam 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 SS 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), thus, transport of Fe and/or O ions through this layer is relatively quick process and its growth is controlled by the oxygen flux  from the (solid or mushy) crust (calculated by the above described diffusion transport model). The SS corrosion model will be numerically realized and implemented in the MO model in the subsequent stages of the Project.

**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

The code CONV was modernized by including a new procedure for solving elliptical equations for the correction of pressure and new developed numerical scheme of the highest order of accuracy for solving of Navier-Stokes equations.

The new procedure for solving elliptical equations with boundary conditions of Neumann for the correction of pressureis based on the modified Richardson iterative method with strongly variable factors using Fast Fourier Transformation algorithm as a preconditioner.

The developed numerical scheme for solving of Navier-Stokes equations is based on a principle of splitting on physical processes. For solving of a convective part of Navier-Stokes equations the new effective scheme for solving of advection equations of higher order and with both low amplitude and dispersing errors was proposed.

Numerical experiments at the choice of optimum turbulence model (algebraic type) are conducted. Among them are approximated turbulence model, algebraic turbulence model (Bolduin-Lomax) and quasi DNS approach.

For simulation of turbulence flows the quasi direct numerical simulation (QDNS) approach and developed algebraic turbulence model were implemented in the CONV code. The applicability of the developed turbulence approach was proved by the extensive validation against the 2D and 3D results of lid-driven flows, flow in tube, the convection in a cavity with the walls supported under different temperature, and convection of a heat-generating fluid. In all cases a good agreement of numerical predictions with experiments and benchmarks was obtained.

With a wide spreading of the multiprocessor computer systems there is a need for development of the parallel version of CFD CONV code. The preliminary parallel version of CONV code was developed for multidimensional modeling of thermal hydraulics processes on the basis of MPI and OpenMP technologies. The outcomes demonstrate increasing of speedup for the parallel version CONV code in comparison with its PC analog.

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). Part #1**

Представлено М.С. Вещуновым на заседании 16th CEG-SAM (Москва, сентябрь 2009)

Presented by M.S. Veshchunov

The progress report on the Project THOMAS is presented. This includes brief general information on the Project organization, main objectives and time schedule. In more details results of Tasks 1, “Development and Improvement of the Physico-Chemical Model for the U-Zr-O Melt Oxidation on the Base of New Crucible Tests”, obtained during 3-4 Quarters are outlined.

Main stages of molten U-Zr-O corium interactions with SS walls are analysed:

During initial transient stage rapid formation of solid, or mushy (depending on oxygen content in the melt), crust controlled by (rapid) heat exchange processes accompanied with mixing of melt, in neglect of (slow) diffusional redistribution of components, take place. This stage can be generally described by thermohydraulic codes (e.g., to be realized in the CONV code).

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 gradient and oxidizing conditions in the melt. During this stage, the following physico-chemical processes simultaneously take place:

* Conversion from mushy to solid crust, accompanied with
* Crust growth,
* Corrosion (oxidation) of SS walls,

which are strictly controlled by oxygen transport through the multilayered structure.

Growth of the solid crust owing 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 base of new FZK crucible tests within the current Project.

Corrosion of SS walls is analyzed using experimental data from the ISTC Project METCOR. The available SVECHA model for stainless steel oxidation in steam 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 SS 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), thus, transport of Fe and/or O ions through this layer is relatively quick process and its growth is controlled by the oxygen flux  from the (solid or mushy) crust (calculated by the above described diffusion transport model).

The SS corrosion model is numerically realized and implemented in the MO model. The new model was tested and then applied to consideration of typical temperature scenarios of tests carried out in the ongoing ISTC Project METCOR.

The model allows interpretation of the main tests observations and qualitatively correctly describes SS 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 SS corrosion kinetics described by the new model using “flowering” mechanism (developed earlier in the SVECHA code for oxidized ZrO2 cladding failure above Zr melting point on the base of the FZK high-temperature tests).

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. **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). Part #2**

Представлено В.В. Чудановым на заседании 16th CEG-SAM (Москва, сентябрь 2009)

Presented by V.V. Chudanov

The progress report on the Project THOMAS is presented. In more details results of Tasks 2, “Development and Improvement of the Unified Thermal Hydraulic Technique (CONV Code) for Simulation of Multiphase Processes in Complex Domains of Convectively Stirred Melt”, obtained during 3-4 Quarters are outlined.

The numerical experiments at the choice of optimum turbulence model (algebraic type) are presented. Among models are considered: 1) approximated turbulence model, 2) algebraic turbulence model (Bolduin-Lomax) and 3) quasi DNS approach.

In our case for a convection of a heat-generating fluid in interesting range of Rayleigh number the approximating turbulence model was proposed and calibrated. The choice of algebraic models is stipulated by conceptual simplicity. They seldom call unexpected numerical difficulties. As the algebraic models are so convenient, it is necessary to abstain from their use only, if the alternative, exceeding them is accessible. However always it is necessary to remember a problem of incompleteness. The algebraic models will well work only for flows, for which they were adjusted in details. Extrapolation outside of the established database, for which the algebraic model was calibrated, does not enough hope.

In the report the results of modernization of CONV code and examples of its validation are submitted on such tests, as: convection in a cavity with the walls with different temperatures and convection of a heat-generating fluid, 3D convection in a lid-driven cavity flow, backward-facing step flow and full turbulent flow of water in a round pipe. The carried out validation of the modified software on the accessible tests demonstrates a good agreement of numerical predictions with experiments.

Also in the report the directions of further works are discussed.

In the report the singularities of realization LES approach in CONV code are briefly presented.

The modeling of a large-scale turbulence is based on a turbulence filtration and in essence this method is more universal, as the immediate restriction on magnitude of Reynolds number does not superimpose.

Let's remark, that the satisfactory exactitude of the closure schemes of for small-scale component of driving is reached only then, when the separation of flow both on small-scale and large-scale components does not render noticeable influence on evolution of large-scale structures.

Obvious shortage of models of a small-scale turbulence is it deterministic character. A casual influence of driving with small-scale on large-scale flow cannot be described by means of such models. As a result the modern turbulence models with scales smaller of a calculated grid step become more complicated.

Such thickening of models is stipulated by desire to achieve an adequate accuracy at a rough calculated grid. As result a universality of obtained models is decreasing.

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

Because of development of computer facilities and appearance of the large computing resources today LES approach is applied more actively in engineering fields.

The preliminary results of testing of the modified version of CONV code on such experimental tests as Backward-facing step flow, T-junction thermal mixing test are simultaneously considered. Also extension CONV code by computing module of magnetic hydrodynamics is brief presented. This module will allow in the future using CONV code for modeling of a skin-layer for needs of LAVA experiments (FZK), which are intended for modeling of molten pool oxidation in new (proposed) crucible tests(1/3). In the report is present a numerical technique for research of influence of high-frequency magnetic hydrodynamics on heating and melting of a corium in 2D statement.