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|  | PROJECT PROPOSAL | # |

## I. Summary Project Information

### 1. Project Title and Taxonomy

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| **Full title:** | Phase relations in corium systems | | | |
| **Short title:** | | PRECOS | | |
| **Technology area:** | | | FIR-EXP, FIR-MOD, FIR-NSS nuclear reactors | |
| **Category of technology development:** | | | | Applied research |

### 2. Project Manager

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| --- | --- | --- | --- | --- | --- | --- | --- | --- |
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| **Title:** | Dr. Sci. (Engineering) | | | | **Position:** | | Department Head | |
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| **City:** | Sosonovy Bor | | | | **Region:** | | Leningrad | |
| **ZIP:** | 188540 | | | | **Country:** | | | Russia |
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### 3. Participating Institutions

#### 3.1. Leading Institution

|  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Short reference:** | | | | | NITI | | | | | | |
| **Full name:** | | | A.P. Alexandrov Research Institute of Technology (NITI) | | | | | | | | |
| **Street address:** | | | | NITI | | | | | | | |
| **City:** | Sosonovy Bor | | | | | | | **Region:** | | Leningrad | |
| **ZIP:** | 188540 | | | | | | | **Country:** | | | Russia |
| **Name of Signature Authority:** | | | | | | | Vasilenko Vyacheslav Andreyevich | | | | |
| **Title:** | Dr.Sci. (Engineering) | | | | | | | **Position:** | | Director General | |
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| **Governmental Agency:** | | | | | | Federal Atomic Energy Agency | | | | | |

#### 3.2. Other Participating Institutions

#### Participant Institution 1

|  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Short reference:** | | | | | ITES OIVT RAS | | | | | | |
| **Full name:** | | | Institute of Thermophysics in Extreme Conditions of the Amalgamated Institute of Hight Temperatures of RAS | | | | | | | | |
| **Street address:** | | | | 13/19, Izhorskaya Str. | | | | | | | |
| **City:** | Moscow | | | | | | | **Region:** | |  | |
| **ZIP:** | 127412 | | | | | | | **Country:** | | | Russia |
| **Name of Signature Authority:** | | | | | | | Zeygarnik Vladimir Albertovich | | | | |
| **Title:** | Dr. Sci. (Engineering), Professor | | | | | | | **Position:** | | Chief Executive | |
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| **Governmental Agency:** | | | | | | Russian Academy of Sciences | | | | | |
| **Sub-manager:** | | | | Sheindlin Mikhail Alexandrovich | | | | | | | |
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### 4. Foreign Collaborators/Partners

#### 4.1. Collaborators

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Institution:** | | | | Forschungszentrum Karlsruhe GmbH | | | | | | |
| **Street address:** | | | | | P.O. Box 3640 | | | | | |
| **City:** | Karlsruhe | | | | | **Region/State:** | | | |  |
| **ZIP:** | 76021 | | | | | **Country:** | | | Germany | |
| **Person:** | | | Walter Tromm | | | | | | | |
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| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Institution:** | | | | Forschungszentrum Karlsruhe GmbH (FZK) | | | | | | |
| **Street address:** | | | | | P.O. Box 3640 | | | | | |
| **City:** | Karlsruhe | | | | | **Region/State:** | | | |  |
| **ZIP:** | 76021 | | | | | **Country:** | | | Germany | |
| **Person:** | | | Alexei Miassoedov | | | | | | | |
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| **Institution:** | | | | EUROPAISCHE KOMISSION, Institut fur Transurane (JRC ITU) | | | | | | |
| **Street address:** | | | | | P.O. Box 2340 (Hermann-Von-Helmholz P1.1) | | | | | |
| **City:** | Karlsruhe | | | | | **Region/State:** | | | |  |
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| **Person:** | | | David Bottomley | | | | | | | |
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| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Institution:** | | | | IRSN/DRS/SEMAR/CEN Cadarache | | | | | | |
| **Street address:** | | | | | Bat 700, BP3, 131115 Cadarache, St. Paul lez Durance | | | | | |
| **City:** | St. Paul lez Durance | | | | | **Region/State:** | | | |  |
| **ZIP:** | F-03108 | | | | | **Country:** | | | France | |
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| **Institution:** | | | | AREVA NP GmbH, NEPR-G | | | | | | |
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| **City:** | Erlangen | | | | | **Region/State:** | | | |  |
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| **Street address:** | | | | | Freyeslebenstr. 1 | | | | | |
| **City:** | Erlangen | | | | | **Region/State:** | | | |  |
| **ZIP:** | 91058 | | | | | **Country:** | | | Germany | |
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| **Institution:** | | | | CEA Grenoble - DTA/CEREM/DEM/SPCM | | | | | | |
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| **Institution:** | | | | FORSCHUNGSZENTRUM ROSSENDORF (FZR) | | | | | | |
| **Street address:** | | | | | Bautzner landstr. 128 | | | | | |
| **City:** | Dresden | | | | | **Region/State:** | | | |  |
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| **Person:** | | | Eberhard Altstadt | | | | | | | |
| **Title:** | | Doctor | | | | **Position:** | | Head of Department | | |
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| **Institution:** | | | | CEA Cadarache - DEN/DTN/STRI | | | | | | |
| **Street address:** | | | | | Batiment 708 | | | | | |
| **City:** | Saint Paul lez Durance | | | | | **Region/State:** | | | |  |
| **ZIP:** | 13108 | | | | | **Country:** | | | France | |
| **Person:** | | | Pascal Piluso | | | | | | | |
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| **Institution:** | | | | IRSN Cadarache - DRS/SEMAR/CEN | | | | | | |
| **Street address:** | | | | | Batiment 700 | | | | | |
| **City:** | Saint Paul lez Durance | | | | | **Region/State:** | | | |  |
| **ZIP:** | 13108 | | | | | **Country:** | | | France | |
| **Person:** | | | Florian Fichot | | | | | | | |
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| **E-mail:** | | | florian.fichot@irsn.fr | | | | | | | |

#### 4.2. Partners

No

### 5. Project Duration

36 months

### 6. Project Location and Equipment

|  |  |
| --- | --- |
| **Institution** | **Location, Facilities and Equipment** |
| **Leading Institution** | Address of equipment location:  Bldg 12 (assembling hall), Bldg 11 (rooms. 405,406) of LSK «Radon» in Sosnovy Bor, 188540 Leningrad Region, Russia.  Equipment:  RASPLAV-2, RASPLAV-3 and RASPLAV-4 experimental facilities employing the method of induction melting in the cold crucible (IMCC) for producing molten prototypic corium heated up to 3300 ºC in a neutral or oxidizing atmosphere (HF generator, induction furnaces, protection and auxiliary technological systems). The RASPLAV-2 facility is employed for the tests with the oxidized and suboxidized oxidic systems; RASPLAV-3 is used for the tests with metal-oxidic systems, while RASPLAV-4 has been designed for the tests with silica-containing systems. Data acquisition complex that comprises detectors and sensors for measuring electric parameters of the generator, flow-rate, temperature, etc. Devices and facilities for physicochemical analyses (mass-spectrometer, X-ray diffractometers and spectrometers, Galakhov microfurnace, chromatograph, etc.). SETARAM thermoanalyzer for the differential thermal analysis, calorimetry and thermogravimetry. Computers and office equipment. |
| **Participant Institution 1** | Address of equipment location:  13/19, Izhorskaya Str., Bldg. 1B-36, Rooms 3-4, 3-13, 3-14, 127412 Moscow, Russia.  Equipment:  The tests with the studied specimens employ a powerful CW ytterbium fiber laser with time programmed power and other lasers, e.g., LTN-103, LK-200-OV and YLR-1500. For the specimen surface observation, high-speed videorecording is used. The analyses of microstructure and elemental composition of the initial and tested specimens are made using the Hitachi S405A scanning electron microscope, Stereoscan S4-10 scanning electron microscope and Cameca SX100 X-ray microanalyzer. The X-ray diffractometry is carried out using DRON-3, DRON-2 and DRON-0.5 X-ray diffractometers.  Multiwave pyrometry. Computers and office equipment. |

### 7. Total Project Effort

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| --- | --- |
| **Total number of participants** | 55 |
| **Number of weapon scientists and engineers** | 28 |
| **Total project effort (person\*days)** | 22192 |
| **Total project effort of weapon scientists and engineers (person\*days)** | 11110 |

### 8. Financial Information

#### 8.1. Estimated Project Costs

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| --- | --- |
| **Estimated total cost of the project (US $)** | 995610 |
| *Including:* |  |
| **Payments to Individual Participants** | 659170 |
| **Equipment** | 235280 |
| **Materials** | 13920 |
| **Other Direct Costs** | 20000 |
| **Travel** | 25240 |
| **Overhead** | 42000 |

#### 8.2. Funding Sources

|  |  |
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| **Estimated total cost of the project (US $)** | 995610 |
| *Financial Sources:* |  |
| **Requested from the ISTC** | 995610 |
| **Other financial source 1** | 0 |
| *Non-Financial Sources:* |  |
| **Non-financial source:** NITI | 200000 |
| **Non-financial source:** OIVT RAS | 50000 |

### 9. Summary of the project

The general objective of the proposed project is to ensure NPP reactor safety in case of a severe accident with core meltdown, and optimal designing of the melt localization devices by means of enhancing precision of thermodynamic calculations of phase conditions and transformations in multicomponent corium systems.

Specific subject of the project is the experimental investigation of phase diagrams of oxidic and metal-oxidic corium systems which form as the result of core meltdown and interaction of melt with construction and structural materials of the reactor, concrete shaft and core catcher.

The modern practice of justifying safety of reactor facilities in case of a severe accident is to a significant extent based on the coupled thermalhydraulic and thermodynamic modeling of the involved high-temperature process. Thermodynamic modeling of multicomponent melts employs specialized numerical codes (e.g., GEMINI-2) and program-specific databases (e.g., NUCLEA-06) created on the basis of experimental data the volume of which is still insufficient for reliable reactor application.

A significant number of investigations was devoted to experimental studies of corium phase diagrams. Among the recent ones there should be mentioned such EU projects as ECOSTAR, COLOSS, ENTHALPY, CIT and SARNET (the proposed project performers participated in the three former ones), as well as the ISTC project # 1950.2 CORPHAD, entirely realized by the proposed project performers.

For instance, the said European projects have helped to optimize the following diagrams: UO2-ZrO2; UO2-ZrO2-FeO-Cr2O3; Fe2O3-ZrO2; Fe2O3-UO2. The CORPHAD project (completed in November 2006) had yielded new data on phase diagrams of other systems of relevance to the reactor application, and concomitant information of importance for understanding mechanisms of physicochemical processes and for increasing precision of modeling thermodynamics and thermochemistry of multicomponent corium systems:

* The binary oxidic systems UO2-FeO, ZrO2-FeO, Fe2O3(Fe3O4)-SiO2 and Fe3O4-SiO2 have been investigated. Tliq/Tsol concentration dependencies within a broad range have been determined along with the eutectic point coordinates and the limits of components’ solubility in the solid phase. The obtained results allowed optimizing the NUCLEA database.
* A limited domain of the SiO2-UO2 binary system has been studied, the miscibility gap boundary and monotectic temperature evaluated.
* A study has been performed to determine coordinates of eutectic points of the ternary oxidic system UO2±x-ZrO2-FeOy under low oxyge potential of the system (in an inert atmosphere) and in the oxidizing atmosphere (air).
* Tliq and Tsol, as well as compositions of the liquids coexisting in the miscibility gap have been determined for a range of compositions of ternary metal-oxidic systems U-Zr-O, Zr-Fe-O and U-Fe-O in the low oxygen concentrations domain.
* Tliq has been determined for the composition of a multicomponent prototypic corium mixture specified by the collaborators.
* Extensive studies aimed at developing thermal analysis methodology have been carried out.
* The facilities fit for realization of new analytical methods have been created.

The newly invited participants from IVT RAS have also developed a new method and designed a facility for phase diagram studies by means of laser-induced heating (Laser pulse method), the application of which has yielded new experimental data on phase diagrams of UO2-ZrO2, UO2-Zr and U-O.

The obtained results were used for optimizing the NUCLEA database and raising precision of modeling in-vessel thermodynamic behaviour of corium during a severe accident with core melting. The main results of the preformed studies have been published in the following papers and presentations:

- Lopukh D., Bechta S., Pechenkov A., Vitol S., Hellmann S., Fischer M., Froment K., Duret B., Seiler J. New Experimental Results on the Interaction of Molten Corium with Core Catcher Material // 8th International Conference on Nuclear Engineering, ICONE-8179, April 2-6, 2000, Baltimore, MD, USA.

- Mezentseva L.P., Popova V.F., Almjashev V.I., Lomanova N.A., Ugolkov V.L., Bechta S.V., Khabensky V.B., Gusarov V.V. Phase and chemical transformations in the SiO2-Fe2O3(Fe3O4) system at different partial pressure of oxygen // J. of Inorganic Chemistry, 2006, V. 51, No. 1, p. 1-8.

- Bechta S.V., Krushinov E.V., Almjashev V.I., Vitol S.A., L.P., Petrov Yu.B., Lopukh D.B., Khabensky V.B., Barrachin M., Hellmann S., Gusarov V.V. Phase relations in the ZrO2-FeO system// J. of Inorganic Chemistry, 2006, V. 51, No. 2, p. 367-374.

- Bechta S.V., Krushinov E.V., Almjashev V.I., Vitol S.A., Mezentseva L.P., Petrov Yu.B., Lopukh D.B., Khabensky V.B., Barrachin M., Hellmann S., Froment K., Fischer M., Tromm W., Bottomley D., Defoort F., Gusarov V.V., Phase diagram of the ZrO2-FeO system // J. Nucl. Mater., 348 (2006), 114-121.

- Mezentseva L.P., Popova V.F., Almjashev V.I., Lomanova N.A., Ugolkov V.L., Bechta S.V., Khabensky V.B., Barrachin M., Hellmann S., Gusarov V.V. Phase diagrams of the SiO2-Fe2O3(Fe3O4) systems in different gas atmospheres // J. Europ. Ceram. Soc., 2006, in press.

- Bechta S.V., Khabensky V.B., Granovsky V.S., Krushinov E.V., Vitol S.A., Gusarov V.V., Almjashev V.I., Mezentseva L.P., Petrov Yu.B., Lopukh D.B., Fischer M., Bottomley D., Tromm W., Barrachin M., Altstadt E., Piluso P., Fichot F., Hellmann S., Defoort F., CORPHAD and METCOR ISTC projects // The first European Review Meeting on Severe Accident Research (ERMSAR-2005), Aix-en-Provence, France, 14-16 November, 2005.

- Bechta S.V., Krushinov E.V., Almjashev V.I., Vitol S.A., Mezentseva L.P., Lopukh D.B., Petrov Yu.B., Khabensky V.B., Barrachin M., Hellmann S., Froment K., Fischer M., Tromm W., Bottomley D., Defoort F., Gusarov V.V., Phase diagram of the UO2-FeO1+x system // J. Nucl. Mater., 362 (2007) 46-52

- Bechta S.V., Krushinov E.V., Almjashev V.I., Vitol S.A., Mezentseva L.P., Petrov Yu.B., Lopukh D.B., Lomanova N.A., Khabensky V.B., Barrachin M., Hellmann S., Froment K., Fischer M., Tromm W., Bottomley D., Gusarov V.V. Phase transformations in the binary section of the UO2-FeO-Fe system // Radiochemistry, 2007, V. 49, No. 1, p. 20-24.

- Manara D., Sheindlin M. and Levis M. Advances in Measurements of the Melting Transition in Non-Stoichiometric UO2 // Int. J. of Thermophysics, vol. 25, No. 2 (2004), p. 533-545.

- Manara D., Pflieger R. and Sheindlin M. Advances in the Experimental Determination of the Uranium – Oxygen Phase Diagram at High Temperature // Int. J. of Thermophysics, vol. 20, ¹ 4, July 2005, p. 1193-1206.

- Pflieger R., Sheindlin M. And Colle J.-Y., Thermodynamics of Refractory Nuclear Materials Studied by Mass Spectrometry of Laser-Produced Vapors // Int. J. of Thermophysics, vol. 26, ¹ 4, July 2005, p. 1075-1093.

At the same time, the large number of the little-investigated systems, laboriousness and complexity of performing tests with and posttest analyses of the high-temperature corium, as well as the limited time for realization of the ISTC CORPHAD project prevented a comprehensive study of phase diagrams of the systems that form during a severe accident, have relevance to the reactor application and are used for justifying safety of reactor facilities.

Among these little-studied systems are:

- Binary and ternary oxidic systems (CaO-UO2, CaO-FeO, SiO2-UO2, UO2-FeO-SiO2, UO2-FeO-CaO, ZrO2-FeO-SiO2, ZrO2-FeO-CaO) containing components of concretes and sacrificial materials, i.e. of importance for modeling the interaction of corium with materials of the concrete shaft and core catcher at the ex-vessel stage of a severe accident development. The SiO2–containing systems should be specially mentioned, as their high viscosity and low electroconductivity make their experimental investigation problematic. Still, they are very important for modeling the ex-vessel corium from a series of power reactors, including such modern ones as EPR.

- Metal-oxidic systems U-Zr-Fe-O with different concentrations of components, especially in the miscibility gap.

- Multicomponent mixtures representing prototypic ex-vessel corium.

The said systemns are to be studied in the proposed project.

The main results of the project should be the following experimentally determined main characteristics:

* Tliq and Tsol concentration dependencies;
* Coordinates of characteristic points, such as eutectic, dystectic, etc.;
* Limits of components solubility in the solid phase;
* Compositions of the liquids coexisting in the miscibility gap.

The data generated in the course of the project implementation will be used for:

* Replenishing databases with the missing or specified experimental information concerning phase diagrams of the oxidic and metal-oxidic corium systems;
* Refining the calculated thermodynamic models, including the sphere of modeling stratification and the quasiequilibrium states under thermogradient conditions;
* Verifying thermodynamic numerical codes that model phase diagrams of multicomponent systems which form as the result of interaction between the molten core and structural and construction materials of the reactor, concrete shaft and core catcher.;
* Justifying and enhancing safety of the existing and new NPP designs with VVER, PWR and BWR reactors.

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|  | PROJECT PROPOSAL | # |

## II. Detailed Project Information

### 1. Introduction and Overview

The general objective of the proposed project is to ensure NPP reactor safety in case of a severe accident with core meltdown, and optimal designing of the melt localization devices by means of enhancing precision of thermodynamic calculations of phase conditions and transformations in multicomponent corium systems.

Specific subject of the project is the experimental investigation of phase diagrams of oxidic and metal-oxidic corium systems which form as the result of core meltdown and interaction of melt with construction and structural materials of the reactor, concrete shaft and core catcher.

The modern practice of justifying safety of reactor facilities in case of a severe accident is to a significant extent based on the coupled thermalhydraulic and thermodynamic modeling of the involved high-temperature process. Thermodynamic modeling of multicomponent melts employs specialized numerical codes (e.g., GEMINI-2) and program-specific databases (e.g., NUCLEA-06) created on the basis of experimental data the volume of which is still insufficient for reliable reactor application.

A significant number of investigations was devoted to experimental studies of corium phase diagrams. Among the recent ones there should be mentioned such EU projects as ECOSTAR, COLOSS, ENTHALPY, CIT and SARNET (the proposed project performers participated in the three former ones), as well as the ISTC project # 1950.2 CORPHAD, entirely realized by the proposed project performers.

For instance, the said European projects have helped to optimize the following diagrams: UO2-ZrO2; UO2-ZrO2-FeO-Cr2O3; Fe2O3-ZrO2; Fe2O3-UO2. The CORPHAD project (completed in November 2006) had yielded new data on phase diagrams of other systems of relevance to the reactor application, and concomitant information of importance for understanding mechanisms of physicochemical processes and for increasing precision of modeling thermodynamics and thermochemistry of multicomponent corium systems:

* The binary oxidic systems UO2-FeO, ZrO2-FeO, Fe2O3(Fe3O4)-SiO2 and Fe3O4-SiO2 have been investigated. Tliq/Tsol concentration dependencies within a broad range have been determined along with the eutectic point coordinates and the limits of components’ solubility in the solid phase. The obtained results allowed optimizing the NUCLEA database.
* A limited domain of the SiO2-UO2 binary system has been studied, the miscibility gap boundary and monotectic temperature evaluated.
* A study has been performed to determine coordinates of eutectic points of the ternary oxidic system UO2±x-ZrO2-FeOy under low oxyge potential of the system (in an inert atmosphere) and in the oxidizing atmosphere (air).
* Tliq and Tsol, as well as compositions of the liquids coexisting in the miscibility gap have been determined for a range of compositions of ternary metal-oxidic systems U-Zr-O, Zr-Fe-O and U-Fe-O in the low oxygen concentrations domain.
* Tliq has been determined for the composition of a multicomponent prototypic corium mixture specified by the collaborators.
* Extensive studies aimed at developing thermal analysis methodology have been carried out.
* The facilities fit for realization of new analytical methods have been created.

The newly invited participants from IVT RAS have also developed a new method and designed a facility for phase diagram studies by means of laser-induced heating (Laser pulse method), the application of which has yielded new experimental data on phase diagrams of UO2-ZrO2, UO2-Zr and U-O.

The obtained results were used for optimizing the NUCLEA database and raising precision of modeling in-vessel thermodynamic behaviour of corium during a severe accident with core melting. The main results of the preformed studies have been published in the following papers and presentations:

- Lopukh D., Bechta S., Pechenkov A., Vitol S., Hellmann S., Fischer M., Froment K., Duret B., Seiler J. New Experimental Results on the Interaction of Molten Corium with Core Catcher Material // 8th International Conference on Nuclear Engineering, ICONE-8179, April 2-6, 2000, Baltimore, MD, USA.

- Mezentseva L.P., Popova V.F., Almjashev V.I., Lomanova N.A., Ugolkov V.L., Bechta S.V., Khabensky V.B., Gusarov V.V. Phase and chemical transformations in the SiO2-Fe2O3(Fe3O4) system at different partial pressure of oxygen // J. of Inorganic Chemistry, 2006, V. 51, No. 1, p. 1-8.

- Bechta S.V., Krushinov E.V., Almjashev V.I., Vitol S.A., L.P., Petrov Yu.B., Lopukh D.B., Khabensky V.B., Barrachin M., Hellmann S., Gusarov V.V. Phase relations in the ZrO2-FeO system// J. of Inorganic Chemistry, 2006, V. 51, No. 2, p. 367-374.

- Bechta S.V., Krushinov E.V., Almjashev V.I., Vitol S.A., Mezentseva L.P., Petrov Yu.B., Lopukh D.B., Khabensky V.B., Barrachin M., Hellmann S., Froment K., Fischer M., Tromm W., Bottomley D., Defoort F., Gusarov V.V., Phase diagram of the ZrO2-FeO system // J. Nucl. Mater., 348 (2006), 114-121.

- Mezentseva L.P., Popova V.F., Almjashev V.I., Lomanova N.A., Ugolkov V.L., Bechta S.V., Khabensky V.B., Barrachin M., Hellmann S., Gusarov V.V. Phase diagrams of the SiO2-Fe2O3(Fe3O4) systems in different gas atmosphere // J. Europ. Ceram. Soc., 2006, in press.

- Bechta S.V., Khabensky V.B., Granovsky V.S., Krushinov E.V., Vitol S.A., Gusarov V.V., Almjashev V.I., Mezentseva L.P., Petrov Yu.B., Lopukh D.B., Fischer M., Bottomley D., Tromm W., Barrachin M., Altstadt E., Piluso P., Fichot F., Hellmann S., Defoort F., CORPHAD and METCOR ISTC projects // The first European Review Meeting on Severe Accident Research (ERMSAR-2005), Aix-en-Provence, France, 14-16 November, 2005.

- Bechta S.V., Krushinov E.V., Almjashev V.I., Vitol S.A., Mezentseva L.P., Lopukh D.B., Petrov Yu.B., Khabensky V.B., Barrachin M., Hellmann S., Froment K., Fischer M., Tromm W., Bottomley D., Defoort F., Gusarov V.V., Phase diagram of the UO2-FeO1+x system // J. Nucl. Mater., 362 (2007) 46-52

- Bechta S.V., Krushinov E.V., Almjashev V.I., Vitol S.A., Mezentseva L.P., Petrov Yu.B., Lopukh D.B., Lomanova N.A., Khabensky V.B., Barrachin M., Hellmann S., Froment K., Fischer M., Tromm W., Bottomley D., Gusarov V.V. Phase transformations in the binary section of the UO2-FeO-Fe system // Radiochemistry, 2007, V. 49, No. 1, p. 20-24.

- Manara D., Sheindlin M. and Levis M. Advances in Measurements of the Melting Transition in Non-Stoichiometric UO2 // Int. J. of Thermophysics, vol. 25, No. 2 (2004), p. 533-545.

- Manara D., Pflieger R. and Sheindlin M. Advances in the Experimental Determination of the Uranium – Oxygen Phase Diagram at High Temperature // Int. J. of Thermophysics, vol. 20, ¹ 4, July 2005, p. 1193-1206.

- Pflieger R., Sheindlin M. And Colle J.-Y., Thermodynamics of Refractory Nuclear Materials Studied by Mass Spectrometry of Laser-Produced Vapors // Int. J. of Thermophysics, vol. 26, ¹ 4, July 2005, p. 1075-1093.

At the same time, the large number of the little-investigated systems, laboriousness and complexity of performing tests with and posttest analyses of the high-temperature corium, as well as the limited time for realization of the ISTC CORPHAD project prevented a comprehensive study of phase diagrams of the systems that form during a severe accident, have relevance to the reactor application and are used for justifying safety of reactor facilities.

Therefore, in spite of the performed research, experimental data on phase diagrams are still deficient. Especially it refers to the systems with low oxygen potential and to those containing materials of the ex-vessel constructions. The shortage of experimental data is determined by the following factorsas follows:

* Difficulties related to experimental research on high-temperature (up to 3300 K) reactive molten corium. Only a small number of expperimental facilities are fit for such research, thus the number of the performed tests is limited;
* The use of new structural and construction materials in the NPP designs under development. These include a new class of ‘sacrificial’ materials which are used for controlling a severe accident at the ex-vessel stage;
* Identification of new phenomena intrinsic to the in- and ex-vessel stages of a severe accident, which determine the structure and characteristics of a molten corium pool. For example, this is the extraction of U and Zr from the suboxidized molten corium by molten steel – the effect that was discovered in the tests performed on the RASPLAV-3 facility in the framework of the OECD/MASCA project and had been predicted earlier [Hofmann, 1976], [Parker, 1982] and [Gueneau, 1999];
* Methodological difficulties related to the identification of the composition of the liquids (of oxygen escpecially) that coexist in the miscibility gap.

The results expected from the proposed project should fill the gap in experimental data on phase diagrams of the little-studied corium systems of importance for the reactor application..

Among these little-studied systems are:

- Binary and ternary oxidic systems (CaO-UO2, CaO-FeO, SiO2-UO2, UO2-FeO-SiO2, UO2-FeO-CaO, ZrO2-FeO-SiO2, ZrO2-FeO-CaO) containing components of concretes and sacrificial materials, i.e. of importance for modeling the interaction of corium with materials of the concrete shaft and core catcher at the ex-vessel stage of a severe accident development. The SiO2–containing systems should be specially mentioned, as their high viscosity and low electroconductivity make their experimental investigation problematic. Still, they are very important for modeling the ex-vessel corium from a series of power reactors, including such modern ones as EPR.

- Metal-oxidic systems U-Zr-Fe-O with different concentrations of components, especially in the miscibility gap.

- Multicomponent mixtures representing prototypic ex-vessel corium.

The experimental matrix for the PRECOS project (see Tab. Below) has been jointly developed by the project performers and collaborators, and coordinated at the 11th Meeting of the Contact Expert Group on Severe Accident Management (CEG-SAM).

Experimental matrix

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Task** | **Composition** | **Atmosphere** | **Test objective** | **Method of determination** | **Priority** | **Points number** |
| 1 | Individual compositions in the U-Zr-Fe-O system | Argon | Tliq, Tsol, tie-lines in the miscibioity gap | VPA IMCC1), DTA2), HTM3), Galakhov microfurnace, PLH4) | 1 | 6 |
|  | ZrO2-FeOy | Air and mixtures with controlled partial pressure of О2 | Tliq, Tsol, solubility limits |  | 2 | 3 |
| 2 | UO2-SiO2 |  | Tliq, Tsol, solubility limits, eutectic point, tie-lines in the miscibioity gap |  | 1 | 7 |
|  | CaO-UO2 |  | Tliq, Tsol, solubility limits | VPA IMCC, DTA, HTM, Galakhov microfurnace | 1 | 7 |
| 3 | UO2-FeO-SiO2 | Argon | Tliq, Tsol, solubility limits, tie-lines in the miscibioity gap, ternary eutectic point |  | 1 | 10 |
|  | UO2-FeO-CaO |  | Tliq, Tsol, solubility limits |  | 1 | 10 |
|  | ZrO2-FeO-SiO2 |  | Eutectic point | Equilibrium crystallization during IMCC,  SEM/EDX of the eutectic | 2 | 2 |
|  | ZrO2-FeO-CaO |  |  |  | 2 | 2 |
| 4 | Multicomponent prototypic corium | Argon or air | Tliq | VPA IMCC | 2 | 3 |

1) Induction melting in the cold crucible with visual polythermal analysis

2) Differential thermal analysis

3) High-temperature microscopy

4) Pulsed laser heating

### 2. Expected Results and Their Application

The Project belongs to the applied research category. The main results of the project should be the following experimentally determined main characteristics:

* Tliq and Tsol concentration dependencies;
* Coordinates of characteristic points, such as eutectic, dystectic, etc.;
* Limits of components solubility in the solid phase;
* Compositions of the liquids coexisting in the miscibility gap.

The findings from the project will be used for:

* Replenishing databases with the missing or specified experimental information concerning phase diagrams of the oxidic and metal-oxidic corium systems;
* Refining the calculated thermodynamic models, including the sphere of modeling stratification and the quasiequilibrium states under thermogradient conditions;
* Verifying thermodynamic numerical codes that model phase diagrams of multicomponent systems which form as the result of interaction between the molten core and structural and construction materials of the reactor, concrete shaft and core catcher.;
* Justifying and enhancing safety of the existing and new NPP designs with VVER, PWR and BWR reactors.

2.1. Sustainability Implementation Plan

2.1.1. Results to be promoted

None

2.1.2. Uniqueness of results

The project should yield the still missing experimental data on phase diagrams of high importance for the reactor application.

2.1.3. Demand for results

The project results can be of interest to the research institutions and design engineering firms working in the field of designing and substantiating safety of NPP with VVER, PWR and BWR reactors, as well as to the research organizations engaged in physical chemistry, material science and high-temperature technologies.

2.1.4. Expected income

Not expected

2.1.5. IPR situation

Governed by the Laws of the Russian Federation and the ISTC Model Project Agreement

2.1.6. Additional developments

Not required

2.1.7. Plan of implementation

Experimental and methodological grounds for the research on high-temperature uranium-bearing melts.

2.1.8. Additional licenses or permits

Not required

2.1.9. Business network

Not planned

### 3. Meeting ISTC Goals and Objectives

The project will be implemented within 36 months by 55 participants, of which 28 persons have been previously involed in weapons development.

The work will be performed by the Leading Institution – the A.P. Alexandrov Research Institute of Technology (NITI) of the Russian Atomic Energy Agency, and by the Participant Institution 1 – ITES OIVT RAS.

The present project will:

- allow the specialists, previously involved in weapons development, to redirect their skills to peaceful activities;

- support applied research performed for peaceful purposes, especially in the fields of environment protection, power production and nuclear safety;

- promote integration of Russian scientists into the international scientific community and conserve the scientific capacity of Russia;

- reinforce the transition to market-based economies responsive to civil needs.

Thus, the project meets ISTC goals and objectives completely.

### 4. Scope of Activities

The Project is scheduled for 3 years.

The total funding is 995610 USD.

The tasks envisaged by the proposed project should be solved by means of performing the tests presented in the experimental matrix.

The priority of tests succession, their methodology and specifications, compositions and temperature-concentration domains of the studied systems, as well as the number of experimental points for each system will be discussed and coordinated with collaborators before each test.

According to the experimental matrix, 4 tasks should be implemented.

The objective of all 4 tasts is to obtain the missing experimental data on the metal-oxidic systems of the in-vessel corium and oxidic systems of the ex-vessel corium.

Task 1 - Investigation of individual compositions of the metal-oxydic system U-Zr-Fe-O.

Task 2 - Investigation of binary oxidic systems from the ex-vessel corium components.

Task 3 - Investigation of ternary oxidic systems from the ex-vessel corium components.

Task 4 - Determination of the eutectic composition and temperature for a multicomponent prototypic corium mixture of importance for the reactor application.

Each task includes the following stages: test preparation and performance, primary analysis of the findings, physicochemical analysis, pre- and posttest calculations, and the obtained results analysis.

#### Task 1

|  |  |  |
| --- | --- | --- |
| **Task description and main milestones** | | **Participating Institutions** |
| Investigation of various compositions of the metal-oxidic system U-Zr-Fe-O aimed at determining Tliq, Tsol and tie-lines in the miscibioity gap.  Main stages:  1.1. State of the art review.  1.2. Tests preparation, performance and primary analysis of the findings.  1.3. Posttest physicochemical analysis of samples.  1.4. Pre- and posttest calculations using thermodynamic codes.  Integrated analysis and generalization of the experimental data. | | 1- NITI  2- ITES OIVT RAS |
| **Description of deliverables** | | |
| 1 | A report on the results of studying the U-Zr-Fe-O system. | |
| 2 | The results of Task 1 realization will be discussed in detail at a joint workshop of collaborators and performers. | |

#### Task 2

|  |  |  |
| --- | --- | --- |
| **Task description and main milestones** | | **Participating Institutions** |
| In accordance with the experimental matrix, investigation of the ex-vessel corium binary oxidic systems of importance for the reactor application.  Main stages:  2.1. State of the art review.  2.2. Tests preparation, performance and primary analysis of the findings.  2.3. Posttest physicochemical analysis of samples.  2.4. Pre- and posttest calculations using thermodynamic codes.  Integrated analysis and generalization of the experimental data. | | 1- NITI |
| **Description of deliverables** | | |
| 1 | Progress reports on the results of individual systems studies. | |
| 2 | A report on the results of studying binary oxidic systems. | |
| 3 | Minutes of a meeting with collaborators. | |

#### Task 3

|  |  |  |
| --- | --- | --- |
| **Task description and main milestones** | | **Participating Institutions** |
| In accordance with the experimental matrix, investigation of the ex-vessel corium ternary oxidic systems of importance for the reactor application.  Main stages:  3.1. State of the art review.  3.2. Tests preparation, performance and primary analysis of the findings.  3.3. Posttest physicochemical analysis of samples.  3.4. Pre- and posttest calculations using thermodynamic codes.  Integrated analysis and generalization of the experimental data. | | 1- NITI |
| **Description of deliverables** | | |
| 1 | Progress reports on the results of individual systems studies | |
| 2 | A report on the results of studying ternary oxidic systems. | |

#### Task 4

|  |  |  |
| --- | --- | --- |
| **Task description and main milestones** | | **Participating Institutions** |
| Determination of Tliq for a multicomponent corium system in order to check accuracy of the calculated prediction for the system.  Main stages:  4.1. Pretest calculated prediction for a multicomponent prototypic system.  4.2. Tests preparation, performance and Tliq determination.  4.3. Posttest physicochemical analysis of samples.  4.4. Posttest calculations using thermodynamic codes.  4.5. Integrated analysis and generalization of the experimental data.  4.6. Comparison of the calculated and experimental data. Assessment of the prediction accuracy | | 1- NITI |
| **Description of deliverables** | | |
| 1 | A report on the results of studying multicomponent systems. | |
| 2 | Minutes of a meeting with collaborators. | |

Compositions of the studied systems are specified by collaborators.

Pre- and posttest thermodynamic calculations are to be simultaneously made by collaborators and performers of the GEMINI2 program.

A decision concerning the next test performing or the experimental matrix correcting should be taken after the previous test has been discussed with collaborators.

The number of tests (phase diagram experimental points) should total ~ 50.

In the end of each quarter, a progress report for the reporting period should be submitted. Completion of each task and each year of the project should be marked by a report offering analysis of the results for the whole reporting period. Upon completion of all the work, the final project report should be issued and updated in case it will be recommended by collaborators or the ISTC.

Tasks correlation diagram is given in the figure below.

Tasks 1 – 4 correlation diagram

Experimental matrix

Task 1

Task 2

Task 3

Task 4



### 5. Role of Foreign Collaborators/Partners

This Project envisages the following aspects of cooperation with foreign collaborators:

- Joint development of the experimental matrix and its refinement in the course of the project

- Efficient information exchange during the project implementation

- Discussion of scientific and technical reports (progress, annual, final) with the aim of modifying experimental methodology, considering the proposed improvements to the physicochemical models of interaction

- Cross-check of the project findings by simultaneously making pre- and posttest calculations using the GEMINI2 thermodynamic code, and performing duplicate tests at ITU in Karlsruhe

- Conduction of joint meetings and seminars

- Joint preparation of presentations and papers

### 6. Technical Approach and Methodology

The experimental research in the framework of the CORPHAD project is carried out on the RASPLAV-2, RASPLAV-3 and RASPLAV-4 experimental facilities which permit handling of molten prototypic corium heated up to 3300 K. The RASPLAV-2 facility is employed for the tests with oxidized and suboxidized oxidic systems, RASPLAV-3 is used for the tests with metal-oxidic systems, while RASPLAV-4 has been designed for the tests with the oxidized systems and those containing vitirifying oxides, e.g. silica. Molten corium is produced using the method of induction melting in the cold crucible (IMCC), which is quite promising in terms of phase diagrams investigation (for some systems it is the only possible one), as the presence of the solid phase (lining crust) between the melt and cold crucible prevents crucible-melt mass transfer, ensures melt retention in the crucible and high purity of the melt (at the level of the initial components’ purity.) The IMCC method provides contact-free power input in the melt and internal energy release. The facilities RASPLAV-2 and RASPLAV -3 can be used for producing, respectively, up to 8 an 2 kg of high-temperature molten corium in a neutral above-melt atmosphere, air or steam.

Some experimental studies are carried employ a series of such facilities as the Galakhov microfurnace, high-temperature microscope, derivatographs, and the high-temperature differential thermoanalyzer located at the Institute of Silicate Chemistry of the Russian Academy of Sciences (ISC RAS). These facilities make it possible to investigate constitution phase diagrams up to 2800 K and obtain experimental data of high precision and reliability.

Along with the methods used in the ISTC CORPHAD2 project, the experimental study of the high-temperature behaviour of the metal-oxidic system U-Zr-Fe-O will also employ a method based on the laser-induced heating, which will be performed by another project participant ITES OIVT RAS. This method has been previously employed for studying superstoichiometric urania (Manara & Sheindlin) and the Zr-U-O system (Bottomley & Sheindlin). It will be improved by increasing its information value for determining Tsol and Tliq using the additional high-speed videorecording of the specimen surface.

Therefore, the methods used in phase diagram studies are as follows:

• Visual polythermal analysis in the cold crucible (VPA IMCC)

• Differential thermal analysis (DTA) and Differential scanning calorimetry (DSC)

• Visual polythermal analysis in the Galakhov microfurnace (GM)

• High-temperature microscopy (HTM)

• Specimen laser pulsed heating (LPH)

These methods have been approved in the projects COLOSS, METCOR, CIRMAT, CIT, ENTHALPY, ECOSTAR and OECD/MASCA.

The physicochemical analysis employs the following methods:

1. Elemental analysis

• X-ray fluorescence analysis (XRF)

• Chemical analysis (СhA)

2. Phase analysis

• X-ray diffraction analysis (XRD)

• Energy-dispersive X-ray spectrometry (EDX)

3. Metallography and ceramography (Opt M)

• Optical microscopy

• Scanning electron microscopy (SEM)

4. Oxygen determination using the method of carbothermal reduction of specimens

In order to implement the proposed project, experimental facilities will be modernized and the methods of physicochemical analysis improved, especially those used for oxygen determination in the phases coexisting in the miscibility gap.

### 7. Technical Schedule

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | **Quarter 1** | **Quarter 2** | **Quarter 3** | **Quarter 4** | **Quarter 5** | **Quarter 6** | **Quarter 7** | **Quarter 8** | **Quarter 9** | **Quarter 10** | **Quarter 11** | **Quarter 12** | **Person\***  **days** |
| **Task 1**  Subtasks 1.1-1.4 | Meeting with collaborators | Report |  |  | 1st year report | Meeting with collaborators |  |  |  |  |  | Paper or presentation |  |
| **Person\*days** | 1700 | 1700 | 1700 | 1100 | 1100 | 1100 | 200 | 200 | 200 | 200 | 200 | 200 | 9600 |
| **Task 2**  Subtasks 2.1-2.4 |  |  |  |  |  | Paper or presentation |  |  | Meeting with collaborators |  |  |  |  |
| **Person\*days** |  |  |  | 600 | 500 | 600 | 1000 | 1100 | 900 | 900 |  |  | 5600 |
| **Task 3**  Subtasks 3.1-3.4 |  |  |  |  |  |  |  |  | 2nd year report |  |  | Meeting with collaborators |  |
| **Person\*days** |  |  |  |  |  |  | 592 | 600 | 900 | 900 | 1400 | 1400 | 5792 |
| **Task 4**  Subtasks 4.1-4.6 |  |  |  |  |  |  |  |  |  |  |  | Final report. Paper or presentation |  |
| **Person\*days** |  |  |  |  |  |  |  |  |  |  | 600 | 600 | 1200 |
| **TOTAL** | 1700 | 1700 | 1700 | 1700 | 1600 | 1700 | 1792 | 1900 | 2000 | 2000 | 2200 | 2200 | 22192 |

#### 8. Managerial responsibilities

Task 1 Curator

Dr.Sci. (Phys.-Math.)

Sheindlin Mikhail Alexandrovich

Tasks 2, 3 Curator

Dr.Sci. (Chem.),

Corr. Mem. RAS

Gusarov Victor Vladimirovich

Task 4 Curator

Krushinov Evgeny Vladimirovich

Project manager

Dr.Sci. (Eng.)

Bechta Sevostyan Victorovich

### 9. Financial Information

### 9.1. Estimated Project Costs (US $)

|  |  |
| --- | --- |
| **Estimated total cost of the project** | 995610 |
| **Leading Institution** | 892310 |
| **Participant Institution 1** | 103300 |

#### 9.1.1. Payments to Individual Participants (US $)

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Institution** | **Category I** | **Category II** | **Supporting personnel** | **Total** |
| **Leading Institution** | 349830 | 254400 | 0 | 604230 |
| **Participant Institution 1** | 0 | 52300 | 2640 | 54940 |
| ***Subtotal:*** | | | | 659170 |

#### 9.1.2. Equipment

|  |  |  |
| --- | --- | --- |
| **Institution** | **Equipment description** | **Cost (US $)** |
| **Leading Institution** | Wavelength-dispersive X-ray fluorescent analyzerр MDX 1000 Oxford Instruments. Boc Edwards Magnetron sputtering system. Raytek Marathon MM1MH micropyrometers. Flow meters, spectrometer, computers, furnace, monitors. | 215240 |
| **Participant Institution 1** | Dode laser, optical cbles, optical elements. | 20040 |
| ***Subtotal:*** | | 235280 |

#### 9.1.3. Materials

|  |  |  |
| --- | --- | --- |
| **Institution** | **Materials description** | **Cost (US $)** |
| **Leading Institution** | Chemical utensils, reagents, sieve, filters, thermocouples, etc. | 10840 |
| **Participant Institution 1** | Compressed gases (helium, argon). | 3080 |
| ***Subtotal:*** | | 13920 |

#### 9.1.4. Other Direct Costs

|  |  |  |
| --- | --- | --- |
| **Institution** | **Direct costs description** | **Cost (US $)** |
| **Leading Institution** | Communications, subcontracts, workshops, etc. | 20000 |
| **Participant Institution 1** |  | 0 |
| ***Subtotal:*** | | 20000 |

#### 9.1.5. Travel costs (US $)

|  |  |  |  |
| --- | --- | --- | --- |
| **Institution** | **CIS travel** | **International travel** | **Total** |
| **Leading Institution** | 2000 | 13240 | 15240 |
| **Participant Institution 1** | 2000 | 8000 | 10000 |
| ***Subtotals:*** | 4000 | 21240 | 25240 |

#### 9.1.6. Overhead (US $)

|  |  |  |
| --- | --- | --- |
| **Institution** |  | **Amount** |
| **Leading Institution** |  | 27000 |
| **Participant Institution 1** |  | 15000 |
| ***Subtotal:*** | | 42000 |

### 9.2. Funding Sources

|  |  |
| --- | --- |
| **Estimated total cost of the project (US $)** | 995610 |

#### 9.2.1. Financial Sources

|  |  |  |
| --- | --- | --- |
| **Financial Source** | **Written confirmation (Y/N)** | **Amount**  **(US $)** |
| **Requested from the ISTC** |  | 995610 |
| Other financial source 1 |  | 0 |

#### 9.2.2. Non-Financial Sources

|  |  |  |  |
| --- | --- | --- | --- |
| **Source** | **Short description of contribution** | **Written confirmation (Y/N)** | **Estimated**  **amount**  **(US $)** |
| NITI | Production premises and available equipment. Expenses associated with their maintenance and operation. Transportation services. | Y | 200000 |
| ITES OIVT RAS | Production premises and available equipment. Expenses associated with their maintenance and operation. Transportation services. | Y | 50000 |

#### 9.2.3. Submitted for Funding to Program Beside the ISTC

No

### 10. Intellectual Property Statement

The rights for intellectual property that are generated during the course of the project will be regulated by the laws of **the Russian Federation** and by the procedures, which have been developed by the ISTC.

The general conditions on Intellectual Property Rights as described in the Model Project Agreement will be observed.

### 11. Monitoring and Auditing Statement

In accordance with Article VIII of the ISTC Agreement, project recipients will give to the Center and to each Party which wholly or partly finances a project the right of access to carry out on-site monitoring and audit of all activities of the project. Project agreements will specify the portions of facilities, equipment, documentation, information, data systems, materials, supplies, personnel, and services which will concern the project and therefore will be made accessible for monitoring and audit. Project recipients shall have the right to protect those portions of facilities that are not related to the project.

### 12. Supporting Information

**12.1. Main publications**

1. Lopukh D., Bechta S., Pechenkov A., Vitol S., Hellmann S., Fischer M., Froment K., Duret B., Seiler J. New Experimental Results on the Interaction of Molten Corium with Core Catcher Material // 8th International Conference on Nuclear Engineering, ICONE-8179, April 2-6, 2000, Baltimore, MD, USA.
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