INTERAGENCY AGREEMENT

1. IAA NO.: NRC-HQ-60-16-T-0009

2. ORDER NO.:

3. REQUISITION NO.: RES-16-0425

4. SOLICITATION NO.:

5. EFFECTIVE DATE: 08/24/2016

6. AWARD DATE: 08/24/2016

7. PERIOD OF PERFORMANCE: 09/15/2016 TO 01/31/2020

8. SERVICING AGENCY
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9. DELIVER TO
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WASHINGTON DC 20555-0001

13. LEGISLATIVE AUTHORITY
Energy Reorganization Act of 1974

14. PROJECT ID

15. PROJECT TITLE
FRAPCON AND FRAPTRAN FUEL PERFORMANCE CODE DEVELOP

16. ACCOUNTING DATA
2016-X0200-FEEBASED-60-60D003-17-6-161-1061-253D

17. ITEM NO.	18. SUPPLIES/SERVICES	19. QUANTITY	20. UNIT	21. UNIT PRICE	22. AMOUNT
	The NRC and the DOE Lab Pacific Northwest National Laboratories (PNNL) hereby enter into this Task Order NRC-HQ-60-16-T-0009 under Agreement, NRC-HQ-25-14-D-0001 for the project entitled, "FRAPCON and FRAPTRAN Fuel Performance Code Development and Assessment". The performance period for this agreement shall commence on September 15, 2016 and will expire on January 31, 2020. Consideration and Obligations: Continued ...				

23. PAYMENT PROVISIONS

24. TOTAL AMOUNT: $125,000.00

25a. SIGNATURE OF GOVERNMENT REPRESENTATIVE (SERVICING)

25b. NAME AND TITLE

25c. DATE

26a. SIGNATURE OF GOVERNMENT REPRESENTATIVE (REQUESTING)
Jeffrey R. Mitchell

26b. CONTRACTING OFFICER
JEFFREY R. MITCHELL

26c. DATE 8/24/2016

TEMPLATE - ADM001

SUNSI REVIEW COMPLETE

SEP - 8 2016

ADM002

(a) Authorized Cost Ceiling $1,317,513.00.

(b) The amount presently obligated with respect to this DOE Agreement is $125,000.00. When and if the amount(s) paid and payable to the DOE Laboratory hereunder shall equal the obligated amount, the DOE Laboratory shall not be obligated to continue performance of the work unless and until the NRC Contracting Officer shall increase the amount obligated with respect to this DOE Agreement. Any work undertaken by the DOE Laboratory in excess of the obligated amount specified above is done so at the DOE Laboratory's sole risk.

The following documents are hereby made part of this Agreement:
Attachment No. 1: Statement of Work

NRC CONTRACTING OFFICERS REPRESENTATIVE (COR):
Michelle Bales (Primary) and Ian Porter (Alternate)
PNNL PROJECT MANAGER: April Augustine
Master IAA: NRCHQ2514D0001

00001	Authorized Cost Ceiling Total Obligated Amount$1,317,513.00 Incrementally Funded Amount: $125,000.00	1,317,513.00

This agreement is entered into pursuant to the authority of the Energy Reorganization Act of 1974, as amended (42 U.S.C 5801 et seq.). This work will be performed in accordance with the NRC/DOE Memorandum of Understanding dated November 24, 1998. To the best of our knowledge, the work requested will not place the DOE and its contractor in direct competition with the domestic private sector.

[ ] Fee Recoverable Work
[X] Non-fee Recoverable Work

Notwithstanding the agreement effective dates and period of performance start dates stated elsewhere in the agreement, the effective date of the agreement and start date of the period of performance are the last date of signature by the parties.

Continued ...

IAA NO	ORDER NO	PAGE	OF
NRC-HQ-60-16-T-0009		3	3

The total amount of award: $1,317,513.00. The obligation for this award is shown in box 24.

U.S.NRC
United States Nuclear Regulatory Commission
Protecting People and the Environment

STATEMENT OF WORK (SOW)

NRC Agreement Number	NRC Agreement Modification Number	NRC Task Order Number (If Applicable)	NRC Task Order Modification Number (If Applicable)
NRC-HQ-25-14-D-0001		NRC-HQ-60-16-T-0009	

Project Title
FRAPCON and FRAPTRAN Fuel Performance Code Development and Assessment

Job Code Number	B&R Number	Servicing Agency
TBD		NRC

NRC Requisitioning Office	Period of Performance
RES	Refer to the IAA form.
NRC Form 187, Contract Security and Classification Requirements ☐ Applicable ☒ Not Applicable	☒ Involves Proprietary Information ☐ Involves Sensitive Unclassified
☒ Non Fee-Recoverable	☐Fee-Recoverable (If checked, complete all applicable sections below)
Docket Number (If Fee-Recoverable/Applicable)	**Inspection Report Number (If Fee Recoverable/Applicable)**
Technical Assignment Control Number (If Fee-Recoverable/Applicable)	**Technical Assignment Control Number Description (If Fee-Recoverable/Applicable)**

U.S.NRC
United States Nuclear Regulatory Commission
Protecting People and the Environment

CONTRACTING OFFICER'S REPRESENTATIVE

Contracting Officer's Representative

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Alternate Contracting Officer's Representative

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NRC-FURNISHED PROPERTY/MATERIALS

A number of the tasks listed in Section 4 will utilize information furnished by the NRC. The following information will be provided to Pacific Northwest National Laboratory (PNNL) by the NRC:

- The Symbolic Nuclear Analysis Program (SNAP) code
- APT Plot software
- Halden, Studsvik Cladding Integrity Program (SCIP), Cabri International Project (CIP), and fuel modelling in accident conditions (FUMAC) data for task 3
- Halden and SCIP data for task 4
- Reports listed in the description of task 5
- Results from research programs that have investigated the stated loss-of-coolant accidents (LOCA) phenomena for task 12
- Event reports and modelling details of fuel failure events for task 15
- Results from research programs that have investigated the cladding lift off for task 17

--- End of Executive Summary ---

STATEMENT OF WORK (SOW)

Contents

DESCRIPTION/SPECIFICATIONS/WORK STATEMENT

1.0 BACKGROUND

The NRC has sponsored the development of the FRAPCON and FRAPTRAN fuel performance codes for predicting steady state and transient fuel behavior, respectively.

FRAPCON is a computer code that calculates the steady-state response of light-water reactor fuel rods during long-term burnup. The code calculates the temperature, pressure, and deformation of a fuel rod as functions of time-dependent fuel rod power and coolant boundary conditions. The phenomena modeled by the code include: 1) heat conduction through the fuel and cladding to the coolant; 2) cladding elastic and plastic deformation; 3) fuel-cladding mechanical interaction; 4) fission gas release from the fuel and rod internal pressure; and 5) cladding oxidation. FRAPCON is used to perform independent calculations for regulatory evaluation of fuel performance under normal operation and anticipated operational occurrences (AOOs). The code is also used to generate initial fuel rod conditions that are needed for the evaluation of fuel performance under transient conditions. The documentation for FRAPCON-4 code models, description and assessment were published in "FRAPCON-4.0: A Computer Code for the Calculation of Steady-State, Thermal-Mechanical Behavior of Oxide Fuel Rods for High Burnup, PNNL-19418, Vol.1 Rev.2."

The Fuel Rod Analysis Program Transient (FRAPTRAN) is a computer code that calculates the transient performance of light-water reactor fuel rods during reactor transients and hypothetical accidents such as LOCAs, anticipated transients without scram, and reactivity-initiated accidents (RIA). FRAPTRAN calculates the temperature and deformation history of a fuel rod as a function of time-dependent fuel rod power and coolant boundary conditions. The phenomena modeled by FRAPTRAN include a) heat conduction, b) heat transfer from cladding to coolant, c) elastic-plastic fuel and cladding deformation, d) cladding oxidation, e) fission gas release, and f) fuel rod gas pressure. The documentation for FRAPTRAN-1.5 code models, description and assessment were published in "FRAPTRAN-1.5: A Computer Code for the Transient Analysis of Oxide Fuel Rods, NUREG/CR-7023, Vol. 1 Rev.1 & PNNL-19400, Vol. 1 Rev.1."

2.0 OBJECTIVE

FRAPCON and FRAPTRAN code assessment, development and maintenance drive a significant portion of the fuel research activities and the tools are used in a substantial number of regulatory products. Given the centrality of the FRAPCON and FRAPTRAN codes to the effectiveness of fuel research, it is critical to assess, develop and maintain these tools. NRC is issuing this contract to accomplish assessment, development and maintenance activities for the FRAPCON and FRAPTRAN codes. The work will include activities designed to support a variety of strategic objectives for FRAPCON and FRAPTRAN code development. These objectives are characterized by four main themes:

- Ensuring FRAPCON and FRAPTRAN maintain state-of-the-art features, material properties and fuel performance models.
- Making FRAPCON and FRAPTRAN easier to use and more reliable.
- Developing new capabilities required to perform more sophisticated analysis of in-reactor transient fuel response as well as analysis related to spent fuel storage.
- Supporting an active and engaged peer community through the FRAP User Group.

3.0 SCOPE OF WORK/TASKS

Task 1: Document the Validated Range for the Material Properties and Models used in the FRAPCON and FRAPTRAN

PNNL shall prepare a table to document the validated range for the fuel, cladding and gas material properties in FRAPCON and FRATPRAN. These ranges should include, but not be limited to, the temperatures, U^{235} enrichment, Gd content, Pu content, hydrogen and oxygen content, and pressures (an example for gas properties - outlining the conditions where Helium is treated as a compressible gas may be of interest) that are validated for all fuel, cladding and gas material properties.

PNNL shall develop a second table to document the validated range for each model used in the FRAPCON and FRAPTRAN codes. As an example, many coolant models in FRAPCON are only validated for water under turbulent flow conditions and this shall be documented in this task. A letter report presenting and explaining both tables shall be provided to the COR.

In addition, PNNL shall include notations in the tables to indicate how the validated ranges compare to the range of conditions where the code is being or likely envisioned to be applied. Based on the comparison, PNNL shall develop and document recommendations for future code benchmarks or model improvements. The recommendations shall be provided to the COR in a letter report.

Task 2: Assess Applicability of FRAPCON and FRAPTRAN to Modeling Light Water Reactor Small Modular Reactors with Natural Circulation

PNNL shall assess the readiness of the FRAPCON and FRAPTAN codes to model Light Water Reactor, Small Modular Reactors (SMRs). One area of focus shall be modeling the thermal hydraulic conditions of natural circulation. FRAPCON uses the Dittus-Boelter formulation for determining heat transfer from the cladding to the coolant, but this correlation is valid only for turbulent flows in vertical pipes. The ability to model low flow conditions shall be assessed, and recommendations shall be developed for changes to the code if deemed necessary. PNNL shall provide a letter report documenting the assessment and resulting recommendations to the COR.

Task 3: Perform Targeted Code Assessment Activities

PNNL shall examine the following four properties and models using experimental data from on-going research projects. The COR will provide reports and presentations containing the Halden, (SCIP)[1], CIP,[2] and the International Atomic Energy Agency (IAEA)'s FUMAC data needed for the activities below.

Subtask 3.1: Assess FRAPCON Creep Model
Halden creep experiments in the IFA-699 series have been designed to determine whether or not creep behavior is symmetrical under tensile and compressive loading and reversals and whether or not mechanistic changes occur due to fast fluence effects on clad microstructure. PNNL shall compare the data from these experiments to the FRAPCON creep model.

Subtask 3.2: Assess FRAPCON Fission Gas Release (FGR) Model
SCIP Ramp experiments have been run for short hold time power ramps to simulate AOOs. In addition, some TRANS-RAMP-IV[3] rods were run with transient characteristics similar to AOOs. Finally, recent Halden FGR measurements may be useful. PNNL shall compare pressure and gas spectrometry measurements from these experiments to FRAPCON FGR models.

Subtask 3.3: Assess FRAPTRAN RIA Integral Effects
PNNL shall model new and recently completed RIA tests from the Japan Atomic Energy Agency (JAEA) Nuclear Safety Research Rector (NSRR)[4] program and the CIP Water Loop tests to verify that FRAPTRAN is able to predict parameters of regulatory interest for RIA. This shall include the tests within the NEA/CSNI[5] RIA benchmark exercise (NSRR VA-1, NSRR VA-3, CIP0-1, and a blind calculation of CIP3-1) as well as new tests as they become available.

Subtask 3.4: Assess FRAPTRAN LOCA Integral Effects

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[1] See http://www.studsvik.com/Projects/SCIP-Project-start-page/

[2] See https://www.oecd-nea.org/jointproj/cabri.html

[3] TRANS-RAMP is a project conducted in the R2 test reactor in Sweden to study the pellet clad interaction (PCI)/stress corrosion cracking (SCC) failure propensity of typical PWR test fuel rods, see http://www.oecd-nea.org/tools/abstract/detail/nea-1648/

[4] For additional information about the NSRR test reactor, see https://www.jaea.go.jp/english/04/ntokai/kasokuki/kasokuki_03.html

[5] For additional information on the objectives and projects of the NEA/CSNI, see https://www.oecd-nea.org/nsd/csni/

Halden LOCA experiments in the IFA-650 series includes measurements of many parameters of regulatory interest. PNNL shall model at least one Halden LOCA test each year to verify that FRAPTRAN is able to predict parameters of regulatory interest. PNNL shall also examine FRAPTRAN LOCA interregnal effects through the fuel performance analysis completed as part of NRC's participation in the IAEA's sponsored Coordinated Research Project on FUMAC.

Subtask 3.5: Assess Centerline Temperature Predictions – Halden tests are often instrumented with centerline-temperature thermocouples. PNNL shall compare measurements from select experiments to experimental predictions.

For each of the five subtasks above, PNNL shall provide the results in a letter report to the COR. Based on the outcome of the subtasks, the COR will identify two of the subtasks for which PNNL shall prepare a conference paper, conference presentation or technical journal article.

Task 4: Improve FRAPTRAN Fission Gas Release Model

FRAPTRAN's transient fission gas release model was developed and validated for RIAs. New data from the Halden IFA-650 test series and the Studsvik SCIP-III program has shown that there is a transient release of fission gas during a LOCA that is large enough to influence burst timing and burst strain. The COR will provide relevant data from the Halden and SCIP programs. PNNL shall use the provided information to assess the current fission gas release model by modeling several of the high burnup LOCA tests. If PNNL identifies significant deviations between the current fission gas release model predictions and the measurements in the Halden and SCIP LOCA tests, then PNNL shall propose modification to the fission gas release model to address the deviations. If the COR agrees with the determinations, PNNL shall implement the proposed modifications to the transient to capture the additional fission gas released to the plenum. PNNL shall provide a letter report to the COR, which documents the assessment of the code initially, rationale for any changes to the FGR model, and the assessment of the code following implementation of any changes.

Task 5: Complete Literature Reviews and Perform Subsequent Evaluations

It is critical that FRAPCON and FRAPTRAN maintain state-of-the-art features, material properties and fuel performance models so that they can continue to be relied on as audit tools for licensing reviews. There are four areas that the NRC has identified as important to maintaining state-of-the-art codes; however, it is not clear if there is adequate data to evaluate and address potential deficiencies in these areas. Therefore, PNNL shall complete a literature review in the following four areas (noted as part 1). The COR will provide PNNL with the documents noted in each subtask below. It is expected that PNNL shall be able to identify meaningful data sources in addition to those provided by the COR. This task requires knowledge of fuel behavior research currently being conducted domestically and internationally as well as familiarity with the major peer-reviewed journals where fuel behavior research is published. PNNL shall propose to the COR which literatures reviews provided adequate data. Subsequent to the COR approval of the adequacy of the data, PNNL shall use the data to complete an evaluation of FRAPCON or FRAPTRAN's accuracy for the subject parameter (noted as part 2). For planning purposes, PNNL shall assume that two of the four subtasks will involve the assessment outlined in part 2.

<u>Subtask 5.1: Analyze and Assess FRAPCON EOL Rod Internal Volume Predictions</u>

- Part 1: PNNL shall perform a literature review to identify data sources and experiments which provide rod internal volume data (puncture data) of commercially irradiated rods. Puncture data from commercial rods with IFBA pellets and Gd_2O_3 pellets is of particular high interest. The COR will provide the following reports to be included in the review: N-15/343 SCIP III-198, N-16/005 SCIP III-199, N-16/075 SCIP III-199.
- Part 2: If PNNL determines that there is adequate data, PNNL shall perform an assessment of these data against FRAPCON predictions of rod internal pressure. PNNL shall provide a letter report to the COR to document the assessment.

<u>Subtask 5.2: Analyze and Assess Advanced Cladding Mechanical Properties and Corrosion Behavior</u>

- Part 1: PNNL shall perform a literature review to identify data sources for mechanical properties and corrosion behavior for advanced claddings, including at least Ziron and Low-Tin ZIRLO™. The COR will provide access to information from Halden to be included in the review, including results of IFA-741 or IFA-785. PNNL shall consult with staff in the NRC Office of Nuclear Reactor Regulation before the task begins to determine if additional advanced claddings are also of interest.
- Part 2: If PNNL determines that there is adequate data, PNNL shall perform an assessment of the existing cladding mechanical properties and corrosion models in FRAPCON and FRAPTRAN to determine if design-specific models are needed for these advanced alloys. The evaluation shall include, but is not limited to, the failure and uniform elongation properties, waterside corrosion and creep models. In instances where the current FRAPCON or FRAPTRAN model is not design specific, PNNL shall assess the model for design-specific bias for each alloy. PNNL shall update the FRAPCON assessment database if significant deviations are identified. If only proprietary data is available, the assessment shall still be performed. If the assessment of cladding models against proprietary data indicates that there is a significant bias for advanced claddings, the feasibility and value of developing a proprietary version of the FRAP codes for in-house use shall be evaluated. PNNL shall provide a letter report to the COR to document the assessment.

<u>Subtask 5.3: Analyze and Assess Advanced Fuel Properties and Models</u>

- Part 1: PNNL shall perform a literature review to identify data sources for fuel properties and models for advanced fuels, including at least UO2-Gd2O3 fuel, Chromium-doped UO2 fuel and fuel with integral fuel burnable absorbers (IFBA). The COR will provide access to information from Halden to be included in the review, including results of an IFA-655/629, 716/629 and 720. The COR will consult with staff in the NRC Office of Nuclear Reactor Regulation before the task begins to determine if additional advanced claddings are also of interest.
- Part 2: If PNNL determines that there is adequate data, PNNL shall perform an assessment of the existing fuel properties and models in FRAPCON and FRAPTRAN to determine if design-specific models are needed for these advanced fuels. Specifically, PNNL shall assess the predictions for fuel melting point, thermal conductivity, swelling, FGR behavior and densification. In instances where the current FRAPCON or FRAPTRAN model is not design specific, PNNL shall assess the model for design-specific bias for each fuel design. PNNL shall update the FRAPCON assessment database if significant deviations are identified. If only proprietary data is available, the assessment shall still be performed. If the assessment of fuel properties and models against proprietary data indicates that there is a significant bias for advanced fuels, the feasibility and value of developing a proprietary version of the FRAP codes for in-house use shall be evaluated. PNNL shall provide a letter report to the COR to document the assessment.

<u>Subtask 5.4: Analyze and Provide Recommendations on Transient Fission Gas Release under AOO Conditions</u>

- Part 1: FRAPTRAN's transient fission gas release model was developed and validated for RIAs and Task 4 has been outlined to identify the needed modifications to the transient FGR model to address LOCA transient fission gas release. Discussions with NRC staff also highlighted rod withdrawal errors, control blade maneuvers and load follow operations as situations that may result in transient FGR that is large enough to impact parameters of regulatory interest. PNNL shall perform a literature review to identify integral experiments or separate effects tests that investigate transient fission gas release at conditions expected during an AOO. The COR will provide access to information from Halden to be included in the review, including results of IFA-720.
- Part 2: If PNNL determines that there is adequate data, PNNL shall write a report to define recommendations for possible model improvements that would be needed to account for transient fission gas release during AOOs.

Task 6: Maintain knowledge of state of practice and awareness of meaningful advancement in fuel performance or fuel behavior research findings.

In order to maintain knowledge of the state-of-practice and awareness of meaningful advancement in fuel performance or fuel behavior research findings, PNNL's principle investigators shall attend internationally recognized conferences on the subject of fuel performance or fuel behavior research programs. This includes some combination of the TOPFUEL (for 2016 see http://www5vip.inl.gov/topfuel2016/, location rotates), Light Water Reactor Fuel Performance Meeting (LWRFPM, location rotates), Enlarged Halden Program Group Meeting (Norway) and the Studsvik Cladding Integrity Program Group Meeting (Sweden), Fuel Safety Research Meeting (FSRM, Japan) and DOE/EPRI Advanced Fuel / Accident Tolerant Fuel Update meetings. The annual selection of conferences that PNNL shall attend will be defined by the COR. PNNL shall write a trip report after each meeting, documenting any new data or analytical methodologies presented at the conference, how the data or methodologies compare to those used in FRAPCON and FRAPTRAN, as well as recommendations for utilizing any new data for code assessment or code development activities. As appropriate, in discussion with the COR, PNNL shall write one to two papers per year on code development and assessment activities performed in the last 12 months and submit to conferences and/or journals. PNNL shall provide all presentations and papers to the COR for review at least one week prior to the submittal deadline. In addition, as appropriate and in discussion with the NRC COR, the contractor may write one to two white papers to the Halden and/or SCIP joint programs during the contract term to propose new experiments, develop PIE plans or design experimental instrumentation that will provide particular value to validate analytical tools and methods.

Task 7: Update Input Generators

PNNL shall develop a version of the FRAPCON and FRAPTRAN Excel Input Generators that has the capability to read a simple data file with fuel rod design information. This feature may be used by the NRC staff to quickly generate an input file with proprietary vendor data. PNNL shall also create the Symbolic Nuclear Analysis Program (SNAP)[6] (.med) files for each fuel designs under this task. NRC will provide the SNAP program to PNNL.

Task 8: Update the Input Files for FRAPCON and FRAPTRAN Assessment Cases
PNNL shall create SNAP files for all assessment cases (.med files). SNAP has an import feature that shall read FRAPCON and FRAPTRAN ASCII files and automatically generate .med files. This will make it easier for NRC staff to use and modify the assessment files.

Task 9: Assess FRAPCON/FRAPTRAN Merger

NRC is considering the option of merging the FRAPCON and FRAPTRAN codes into a single fuel performance code, which has advantages over the coupling approach used today. PNNL shall evaluate the effectiveness of FRAPCON or FRAPTRAN for modeling transients on an intermediate time scale, such as those expected during AOOs. The evaluation shall include consideration of the need to model additional phenomena, such as fission gas swelling, fission gas release and cladding creep, in each code by assessing FRAPCON and FRAPTRAN's ability

[6] For additional information about SNAP, see https://www.aptplot.com/snap/index.jsp

to predict stress and strain data generated by integral ramp tests simulating AOO transients. Under this task, PNNL shall write a report, outlining the tasks with estimated time and resources for merging the FRAPCON and FRAPTRAN codes into a single fuel performance code.

Task 10: Ensure Consistency of Models between FRAPCON and FRAPTRAN

Because FRAPCON and FRAPTRAN were originally developed independently, some models are not implemented consistently in the two codes. PNNL shall determine which models are not consistent between codes, and modify the codes so that they are consistent. If models exist for one code but not the other, PNNL shall determine, in discussion with the COR, if adding the model to the other code is appropriate. PNNL shall provide a letter report to the COR to document model inconsistencies and the changes implemented to address the inconsistencies.

Task 11: Ensure Consistency of Material Properties between FRAPCON and FRAPTRAN

Because FRAPCON and FRAPTRAN were originally developed independently, not all material property correlations are implemented the same in the two codes. PNNL shall determine which fuel, cladding and gas properties used in FRAPCON and FRAPTRAN are not consistent between codes, and modify the codes so that they are consistent. If models exist for one code but not the other, PNNL shall determine, in discussion with the COR, if adding the model to the other code is appropriate. PNNL shall provide a letter report to the COR to document model inconsistencies and the changes implemented to address the inconsistencies.

Task 12: Develop Advanced Modeling of LOCA Phenomena

There is a growing interest within the industry to develop best-estimate analysis and address important fuel performance phenomenon mechanistically. There are four LOCA phenomena that the NRC identified as candidates for either a more mechanistic modeling approach or confirmation of best-estimate predictions. The COR will provide PNNL in a letter report, the results from research programs that have investigated these four LOCA phenomena; however it is expected that PNNL shall be able to identify meaningful data sources in addition to those provided by the COR. This requires knowledge of fuel behavior research currently being conducted domestically and internationally as well as familiarity with the major peer-reviewed journals where fuel behavior research is published. It is desirable to approach each of the four LOCA phenomena in three stages where the sub-task begins with data collection (part 1), proceeds to model development only if sufficient data exists (part 2) and concludes with implementation in FRAPTRAN only if the modeling approach is determined to be reasonably best-estimate or mechanistic (part 3). For planning purposes, PNNL should assume that 1 out of the 4 subtasks shall terminate at part 1 and the remaining three will proceed through part 2 and 3. The four LOCA phenomenon are:

<u>Subtask 12.1: Analyze, Propose, and Implement Axial Fuel Relocation New Model</u>

- Part 1: Axial fuel relocation has been shown to occur following the ballooning of cladding during a LOCA. Axial fuel relocation may lead to increased heat load in this area. PNNL shall perform a literature review to identify measurements that quantify the characteristics of relocation, such as the packing fraction of the relocated fuel and cladding temperature rise in the balloon node due to relocated fuel. PNNL shall also review existing relocation models in other transient performance codes.
- Part 2: If PNNL determines that there is adequate data to substantiate an axial fuel relocation model, PNNL shall propose an axial fuel relocation model to the COR by outlining its features, defining how it can be validated, and how it can be integrated into the computational scheme of the FRAPTRAN code. PNNL shall clearly identify the mechanistic and empirical features of the model in the proposal. The proposal for the new model shall be documented in a letter report to the COR.
- Part 3: If the COR determines that PNNL's proposal is viable, PNNL shall add the model to FRAPTRAN. PNNL shall write a report to document the new model, including results of fuel performance predictions compared to measurements for experiments where fuel relocation was observed.

<u>Subtask 12.2: Analyze, Assess, and Modify CRUD[7] Model</u>

- Part 1: The presence of CRUD on fuel rods may have an impact on the initial stored energy of fuel rods prior to a LOCA and on the heat transfer of fuel rods during a LOCA. Currently, FRAPTRAN does not independently model a CRUD layer. However, the appropriateness of this assumption depends on the thickness of the CRUD layer. PNNL shall use NRC event reports to establish typical values of CRUD thickness and conduct a literature review to identify typical values of CRUD thermal conductivity.
- Part 2: PNNL shall perform a sensitivity analysis using FRAPTRAN (initialized with FRAPCON) to assess the effect of CRUD for typical values of CRUD thickness and thermal conductivity. PNNL shall prepare a letter report to document the sensitivity analysis and submit this report to the COR.
- Part 3: If sensitivity analysis demonstrates that cladding temperature predictions are sensitive to typical values of CRUD thickness, then PNNL shall modify the oxide model in FRAPTRAN to distinguish the thickness and thermal properties of ZrO_2 and CRUD. PNNL shall prepare a letter report to describe the changes to the oxide model and the validation cases and submit this report to the COR.

<u>Subtask 12.3: Analyze, Assess, and Implement Improved Rod Ballooning Model with Code Guidance</u>

[7] "CRUD" originated as an acronym for Chalk River Unidentified Deposit, However, today CRUD is a colloquial term for corrosion and wear products (rust particles, etc.) that become radioactive (i.e., activated) when exposed to radiation.

- Part 1: The ballooning model in FRAPTRAN has some restrictions that are not clearly outlined in the FRAPTRAN Code Description, including the fact that ballooning is limited to one node, while the node size is completely up to the user. PNNL shall complete a literature review to identify data sources for balloon length and axial strain profile from LOCA integral tests. PNNL shall evaluate the experimental methodology for each data source to determine if the balloon shape should be considered representative of in-reactor fuel behavior.
- Part 2: If PNNL determines that there is sufficient and appropriate balloon length data available, the implications of small and large ballooning nodes shall be assessed. The assessment shall include evaluation of the impact of balloon node size on the amount of fuel predicted to be available for dispersal from the balloon region.
- Part 3: If PNNL determines that the current ballooning model logic significantly misrepresents scenarios where small or large ballooning nodes are expected, PNNL shall develop and implement an improved balloon model that more accurately reflects the size of the ballooned region. If PNNL determines that no changes to the ballooning model are feasible at this time, PNNL shall develop guidance to be added to the code description document to communicate the ballooning model restrictions.

<u>Subtask 12.4: Implement Developer Option for Consistency with the TRAC/RELAP Advanced Computational Engine (TRACE)[8] Calculation Approach</u>

- The criteria in 10 CFR Part 50, Appendix K, I.A.5[9] specifies that the Baker-Just equation must extend "axially no less than 1.5 inches each way from the location of the rupture". In the TRACE code, there is a re-meshing option that shall adjust the node size at the location where the metal-water reactor occurs to ensure the node is at least 3" in the axial (z) direction. However, FRAPTRAN does not have this capability and the user input axial node length can be smaller than 3". PNNL shall develop and implement a new optional model in FRAPTRAN that re-meshes the balloon node to ensure a minimum of 3" axial node length is used to calculate the metal-water reaction.

Task 13: Implement Improvements and Advancements in Heat Transfer Models in FRAPCON and FRAPTRAN

PNNL shall modify the 1D radial conduction solution in FRAPTRAN to include inner diameter (ID) and outer diameter (OD) oxide thickness and energy generation. Further, there are certain situations, such as during reflood, where 2-D heat transfer may need to be taken into account in the fuel rod. PNNL shall evaluate the effects of axial heat transfer and assess the practicality of

[8] For additional information about the TRACE code, see http://www.nrc.gov/about-nrc/regulatory/research/safetycodes.html#th

[9] http://www.nrc.gov/reading-rm/doc-collections/cfr/part050/part050-appk.html

implementing 2-D heat transfer into the code. If it is shown to have a significant impact, then the thermal solution in FRAPCON and FRATPRAN will be modified to consider 2-D heat transfer. PNNL shall provide a letter report to the COR, documenting the modifications.

Task 14: Implement Combined Fission Gas and Thermal Solutions

Thermal and fission gas production solutions are currently solved and nodalized independently; however, the phenomenon at play are intrinsically linked. For example, there is no feedback of the reduction of the thermal conductivity, associated with the increased porosity, of the HBS structure on the thermal solution. PNNL shall modify the thermal and fission gas solutions in FRAPCON and FRAPTRAN to use the same nodalization and use consistent fuel characteristics. PNNL shall provide a letter report to the COR, documenting the modifications.

Task 15: Perform Evaluation of Fuel Performance during Select Fuel Drying Events

Recently, a number of fuel failures have been detected during the vacuum drying stage of dry storage cask loading. Following the task above, PNNL shall utilize the modified FRAPCON code to model at least two fuel failure events that occurred during drying and evaluate predicted fuel stress and strain to determine if regulatory limits need to be modified in order to prevent a future fuel failure. The COR will provide event reports and modeling details for the fuel failure events. PNNL shall perform the modeling in conjunction with cask thermal analysis results to ensure that the fuel rod boundary conditions are reasonable. PNNL shall provide a letter report to the COR, documenting the modeling results.

Task 16: Develop Hydride Reorientation Model

The contractor shall develop a model to predict the onset and extent of radial hydride reorientation as a function of drying temperature and rod internal pressure. The model shall be used to relate the results to mechanical properties. PNNL shall verify the model using mechanical properties data from irradiated cladding with and without radial hydrides.

Task 17: Develop Inner Diameter (ID) oxidation Growth Model

It is understood that ID oxidation has the potential to influence the gap conductance (among other factors), specifically with respect to emissivity, which is of high importance in ballooning calculations. FRAPCON currently incorrectly uses the cladding OD oxide thickness for calculating gap emissivity, but does not provide this information to FRAPTRAN, which itself uses a default value irrespective of fuel burnup. PNNL shall modify FRAPCON to predict ID oxidation layer growth and pass the value to FRAPTRAN to use in calculations of heat transfer in the fuel/cladding gap during ballooning. PNNL shall document the three part task outlined below in a letter report to the COR.

- Part 1: PNNL shall conduct a literature review to identify data sources for ID oxidation thickness values. The literature review shall also include review of other fuel performance codes to determine if and how ID oxidation is modeled in other fuel performance codes.
- Part 2: If PNNL and the COR agree that there is adequate data to introduce an ID oxidation growth model, then PNNL shall develop and implement the model in FRAPCON.
- Part 3: If a model is developed, PNNL shall modify the FRAPCON-to-FRAPTRAN restart file and re-run all LOCA integral assessment cases with these new values.

Task 18: Implement Regulatory Evaluation Functionality for Cladding Lift-Off

FRAPCON is currently used to evaluate fuel rod performance in over-pressure conditions. However, FRAPCON does not have a cladding lift-off evaluation performed in the Integral Assessment, nor does it produce user messages to indicate that cladding lift-off has occurred or regulatory criteria have been exceeded. The COR will provide results from research programs that have investigated cladding lift-off, in particular data from the Halden lift-off series, IFA-710.X. PNNL shall modify FRAPCON to perform evaluation of cladding-lift off indicators and provide the evaluation results to the user via the Regulatory Information Summary. The contractor shall validate the modified version against available data. PNNL shall document the code modifications and validation in a letter report to the COR.

Task 19: Create New Training and Development Materials

PNNL shall develop on-line tutorials for the FRAPCON/FRAPTRAN User Group. The tutorials shall be made available on the User Group Website. Using a screen capture software such as Camtasia Studio, the tutorials shall demonstrate to users how to do the following:

a) Develop Input Files using the Auto Input Generators
b) Run the codes
c) Use FRAPlot to plot the data
d) Use APT Plot to plot the data
e) Create, run and analyze a case using SNAP
f) How to compile the code on a Windows System using Visual Studio
g) How to compile the code on a Linux System

In addition, the contractor shall develop and make available on the User Group website on-line tutorials on the following advanced topics:

a) How to use the features for modeling refabricated rods in FRAPCON and FRAPTRAN.
b) A review of all "failure limits" included in the FRAPCON and FRATRAN codes.
c) An overview of the ballooning model in FRAPTRAN, explaining how the model works, how to set node size and what areas the user must be careful of.

Task 20: Issue New Code Versions and Documentation

PNNL shall issue FRAPCON-4.1 and FRAPTRAN 2.1 code versions, including the necessary DAKOTA scripts, and the associated code documentation by September 1, 2018, unless an alternative data is discussed and accepted by the COR.

PNNL shall issue FRAPCON-4.2 and FRAPTRAN 2.2 code versions, including the necessary DAKOTA scripts, and the associated code documentation by September 1, 2020, unless an alternative data is discussed and accepted by the COR.

The contractor shall post electronic files for each reference used in the FRAPCON/FRAPTRAN code description and assessment documents on the PNNL SharePoint site.

Each time a new code version is produced, PNNL shall update the Code Description Documents, Material Properties Document and Integral Assessment Documents and these documents shall be issued as NRC NUREG/CR documents. PNNL shall provide Draft versions of the NUREG/CR documents to the COR for a 4 week review prior to PNNL submitting the final document for publication. PNNL shall re-run the integral assessment for all cases, including running FRAPCON to generate new restart files for FRAPTRAN. PNNL shall also modify the Excel-based pre- and post-processors to follow the changes implemented in the new code version.

Task 21: User Group Reporting and Updates

A FRAPCON/FRAPTRAN User Group is organized and administered by PNNL and adds significant value to the code development and maintenance tasks listed above. Periodically, the NRC staff have reporting or tracking obligations related to the code distribution aspect of User Group. In addition, there are occasions where a new NRC requirement or protocol must be implemented in the administration or documentation of the User Group. The contractor shall assist the NRC staff in reporting, tracking and update activities, specifically:

- PNNL shall maintain a list of current Non-Disclosure Agreements (NDA's) and provide the list to the NRC staff when needed.
- PNNL shall respond to NRC inquiries related to the User Group
- PNNL shall complete updates to the User Group Website requested by the NRC staff.

Task 22: Provide On-Call Assistance

On-call assistance represents a continuing effort that should not exceed 10 percent of the total activity for this project. This on-call assistance task is for PNNL to provide technical assistance to NRC staff who use the FRAPCON/FRAPTRAN codes. Technical assistance entails answering and resolving NRC staff questions via phone or email. This assistance is separate from the assistance provided to User Group Members in Task 21.

Activities under this task should be reported in the Monthly Letter Status Report.

4.0 LIST OF DELIVERABLES

Acceptance Criteria: For each deliverable described below, PNNL shall deliver written comments or reports in the required format, quality guidelines, and within the schedule established for COR approval and acceptance. In all cases, only electronic deliverables are requested.

For QA documentation, PNNL shall comply with the "FRAPCON/FRAPTRAN Programming Guidelines" document.

Task/Subtask	Description	Format	Deliverable Date (Months after project start)
1	Letter Report	Word	6 months after award date
2	Letter Report	Word	9 months after award date
3.1, 3.2, 3.3, 3.4	Letter Report	Word	3 years after award date
3	Conference Paper for at least one of the subtasks	Word	3 years after award date
4	Updated source code, associated QA documentation and Letter Report	Source Code, Word	3 years after award date
5.1, 5.2, 5.3, 5.4	Letter Report	Word	1 subtask per year, starting 2 years after award date
6	Trip reports and conference presentations as agreed upon between PNNL and COR. Conference presentation, conference paper or technical journal article, as agreed upon by the COR.	Word, PowerPoint – as appropriate	To be determined based on selected conferences
7	SNAP (.med) files for each fuel design.	.med files	1 year after award date
8	Updated Input files for each Assessment Case	.in files	1 year after

			award date
9	Letter Report	Word	2 years after award date
10	Updated source code, associated QA documentation and Letter Report	Source Code, Word	1 year after award date
11	Updated source code, associated QA documentation and Letter Report	Source Code, Word	3 months after award date
12.1, 12.2, 12.3, 12.4	Updated source code, associated QA documentation and Letter Report	Source Code, Word	3 years after award date
13	Updated source code, associated QA documentation and Letter Report	Source Code, Word	2 years after award date
14	Updated source code, associated QA documentation and Letter Report	Source Code, Word	2 years 6 months after award date
15	Letter Report	Word	2 years 9 months after award date
16	Letter Report	Word	
17 (part 1)	Letter Report	Word	3 years after award date
17 (part 2)	Letter Report	Word	3.5 years after award date
17 (part 3)	If pursued, updated source code, associated QA documentation	Source Code, Word	3.5 years after award date
18	Updated source code, associated QA documentation and Letter Report	Source Code, Word	1 year 9 months after award date
19	Remote accessible video files	At discretion of the COR and compatible with standard browsers in the US, Europe and Asia	1 year 6 months after award date
20	4.1 and 2.1 Code Versions	Source code	1 year after award date
20	Draft NUREG/CR Documentation for 4.1 and 2.1 Code Versions	Word	11 months after award date
20	Final NUREG/CR Documentation for 4.1 and 2.1 Code Versions	Word	1 year after award date

20	4.2 and 2.2 Code Versions	Source code	3 years after award date
20	Draft NUREG/CR Documentation for 4.2 and 2.2 Code Versions	Word	2 years, 11 months after award date
20	Final NUREG/CR Documentation for 4.2 and 2.2 Code Versions	Word	3 years after award date
21	User Group Reporting and Updates	At discretion of contractor	Continuous
22	On-Call assistance	MLSR	Continuous
-	MLSR in accordance with Section F.3. and Attachment 5 of the base contract.		20th of each month

5.0 ESTIMATED LABOR CATEGORIES, KEY PERSONNEL AND LEVELS OF EFFORT

5.1 Labor Categories, Requirements and Key Personnel. Personnel working under this agreement/order shall meet the minimum requirements for experience and education, as follows:

Labor Category	Position Minimum Requirements	Key Personnel* (yes or no)
Senior Key Staff **Kenneth Geelhood**	• Engineering degree • 10 or more years of experience in the modification and further development of the FRAPCON and FRAPTRAN source code, numeric resolution scheme, and code structure. • Demonstrated in-depth knowledge of the FRAPCON and FRAPTRAN models and their supporting database, as well as possession of such a database with the adequate QA in place. This includes knowledge and understanding of the assumptions, simplifications and rationale employed in the empirical models. • Demonstrated in-depth knowledge of the FRAPCON and FRAPTRAN validation database and its data sources, as well as	*Yes*

	possession of such a database with the adequate QA in place. • 10 or more years of experience using the FRAPCON and FRAPTRAN codes. • Demonstrated in-depth knowledge of nuclear fuel behaviour under steady-state and transient regimes, as well as during storage and transportation. • Proven knowledge and extensive experience in writing code language that conforms to the 2015 Fortran standard, including utilizing the functionality of modules, submodules, and class structures. • Knowledge and experience with LaTex, Perl, GNUPlot and GIT.	
Key Staff **Walter Luscher** **Gianluca Longoni**	• Engineering degree • 3 or more years of experience in the modification and further development of the FRAPCON and FRAPTRAN source code, numeric resolution scheme, and code structure. • Demonstrated knowledge of the FRAPCON and FRAPTRAN models and their supporting database. • 3 or more years of experience using the FRAPCON and FRAPTRAN codes. • Demonstrated knowledge of nuclear fuel behaviour under steady-state and transient regimes, as well as during storage and transportation. • Proven knowledge and experience in writing code language that conforms to the 2015 Fortran standard, including utilizing the functionality of modules, submodules, and class structures. • Knowledge and experience with LaTex, Perl, GNUPlot and GIT.	*Yes*

Support Staff	Ability to distribute the FRAPCON and FRAPTRAN codes with NRC oversight. This includes expertise and authority to conduct both the export control and counterintelligence reviews required for distributing materials to foreign organizations.	*No*

6.0 CERTIFICATION AND LICENSE REQUIREMENTS

N/A

7.0 MEETINGS AND TRAVEL

A two-day trip to NRC, Rockville, MD by the principle investigator or other key person to participate in work-related meetings and to present the progress of the work. The NRC anticipates this meeting to occur each fiscal year.

One domestic trip to present papers at conferences are anticipated for each fiscal year. Domestic trips may include TOPFUEL and DOE/EPRI Advanced Fuel / Accident Tolerant Fuel Update meetings and the location will vary. Generally the conferences are 3-4 days and require 5-6 travel days, depending on location. The PNNL staff who attends each conference shall be determined through discussion with the COR.

One to two foreign trips are anticipated each fiscal year. The PNNL staff who attends each conference shall be determined through discussion with the COR. The exact trips will be determined at the start of the fiscal year, but will be one or two of the trips listed below. The selection of trips will vary based on the expected subject material of each conference in the given year:

- Studsvik Cladding Integrity Program (SCIP-III) Program Review Meetings
    - Held twice per year in Sweden.
    - Meeting is typically 3 days. Including travel time, trip is 5-6 days.
- Light Water Reactor Fuel Performance Meeting
    - Held twice out of every 3 years (the third instance in a 3-year period occurs in the US as the TOPFUEL conference)
    - Location rotates between Europe and Asia
    - Meeting is typically 5 days. Including travel time, trip is 6-7 days.
- Halden Program Group (HPG) Meetings
    - Held twice per year in Norway or HPG chairmanship country.
    - Meeting is typically 3 days. Including travel time, trip is 5-6 days
- Fuel Safety Research Meeting (FSRM)

- Held once per year in Japan.
- Meeting is typically 3 days. Including travel time, trip is 5-6 days

All travel requires prior written approval from the COR.

Servicing agency personnel will be authorized travel expenses consistent with the Federal Travel Regulation (FTR) and the limitation of funds specified for the travel within this agreement/order. All travel requires prior written approval from the COR.

Foreign travel for the servicing agency personnel requires a 60-day lead time for NRC approval. For prior approval of foreign travel, the servicing agency shall submit to the COR an NRC Form 445, "Request for Approval of Official Foreign Travel." All foreign travel requires prior written approval from the NRC Executive Director for Operations (EDO).

Travel will be reimbursed in accordance with FAR 31.205-46, "Travel costs" and the General Services Administration's Federal Travel Regulations at: http://www.gsa.gov/portal/content/104790.

No reactor side access is anticipated.

8.0 REPORTING REQUIREMENTS

The servicing agency is responsible for structuring the deliverables to current agency standards. Deliverables shall be submitted free of spelling and grammatical errors and shall conform to requirements stated in this section.

8.1 Monthly Letter Status Report (MLSR)

The servicing agency shall provide a Monthly Letter Status Report which consists of a technical progress report and financial status report. This report will be used by the sponsoring agency to assess the adequacy of the resources utilized by the servicing agency to accomplish the work contained in this SOW and to provide status of the servicing agency progress in achieving tasks and producing deliverables. The report shall include agreement/order summary information, work completed during the specified period, milestone schedule information, problem identification and resolution, travel plans, and staff hour summary. Copies shall be sent to the COR and AMD at ContractsPOT.Resource@nrc.gov.

9.0 REQUIRED MATERIALS, FACILITIES, HARDWARE/SOFTWARE

The following software shall be purchased by PNNL and used in the execution of this contract:

- Intel Parallel Studio XE 2016 Professional Edition: $2,299 per license (http://softwarestore.ispfulfillment.com/Store/Product.aspx?skupart=I23SC9)
- Visual Studio Professional 2015: $499 per license (https://www.visualstudio.com/products/how-to-buy-vs)

Other software purchases may be required to complete the tasks above. Any software purchases shall be approved by the COR prior to purchase.

The servicing agency shall provide the following materials, facilities, hardware, or software required for this agreement/order:

- FRAPCON and FRAPTRAN source code
- All working files and digitized capture of data (both experimental and calculated) associated with the FRAPCON and FRAPTRAN assessment databases. This shall also include a write-up of how the code assessments are performed and what file manipulations are required.
- All input files associated with the FRAPCON and FRAPTRAN assessment databases

10.0 APPLICABLE PUBLICATIONS (CURRENT EDITIONS)

The servicing agency shall comply with the following applicable regulations, publications, manuals, and local policies and procedures:

1. "FRAPCON/FRAPTRAN Programing Guidelines" - outlines the format and structure that all developers must follow when making any change to the source code.
2. FRAPCON/FRAPTRAN Code Maintenance Project Configuration Management and Maintenance Plan (CMMP), PNNL-17477 Rev. 1
3. FRAPCON/FRAPTRAN Software Quality Assurance Plan (SQAP) PNNL-17478 Rev.1

11.0 DATA RIGHTS

The NRC shall have unlimited rights to and ownership of all deliverables provided under this agreement/order, including reports, recommendations, briefings, work plans and all other deliverables. All documents and materials, to include the source codes of any software, produced under this agreement/order are the property of the NRC with all rights and privileges of ownership/copyright belonging exclusively to the NRC. All electronic copies of experimental data, as well as corresponding reports, used for code validation and model development shall also be provided. These documents and materials may not be used or sold by the servicing agency without prior written authorization from the CO. All materials supplied to the NRC shall be the sole property of the NRC and may not be used for any other purpose. This right does not abrogate any other Government rights.