Light Water Reactor Sustainability Program

R&D Plan for RISMC Industry Application #1: ECCS/LOCA Cladding Acceptance Criteria

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April 2016

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EXECUTIVE SUMMARY

The Nuclear Regulatory Commission (NRC) is finalizing a rulemaking change that would revise the requirements in 10 CFR 50.46. In the proposed new rulemaking, designated as 10 CFR 50.46c, the NRC proposes a fuel performance-based equivalent cladding reacted (ECR) criterion as a function of cladding hydrogen content before the accident (pre-transient) in order to include the effects of higher burnup on cladding performance as well as to address other technical issues. A loss of operational margin may result due to the more restrictive cladding embrittlement criteria. Initial and future compliance with the rule may significantly increase vendor workload and licensee costs as a spectrum of fuel rod initial burnup states may need to be analyzed to demonstrate compliance.

The Idaho National Laboratory (INL) has initiated a project, as part of the DOE Light Water Reactor Sustainability Program (LWRS), to develop analytical capabilities to support the industry in the transition to the new rule. This project is called the Industry Application 1 (IA1) within the Risk-Informed Safety Margin Characterization (RISMC) Pathway of LWRS.

The general idea behind the initiative is the development of an Integrated Evaluation Model (IEM). The motivation is to develop a multiphysics framework to analyze how uncertainties are propagated across the stream of physical disciplines and data involved, as well as how risks are evaluated in a LOCA safety analysis as regulated under 10 CFR 50.46c. This IEM is called LOTUS which stands for LOCA Toolkit for US and it represents the LWRS Program’s response to the proposed new rule making.

The focus of this report is to complete an R&D plan to describe the demonstration of the LOCA/ECCS RISMC Industry Application # 1 using the advanced RISMC Toolkit and methodologies. This report includes the description and development plan for a RISMC LOCA tool that fully couples advanced MOOSE tools already in development in order to characterize and optimize plant safety and operational margins. Advanced MOOSE tools that are needed to complete this integrated evaluation model are: RAVEN, RELAP-7, BISON, and MAMMOTH.
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ACRONYMS

AOR       analysis of record
ATWS      anticipated transients without scram
BEPU      best estimate plus uncertainty
CD-A      core design automation
CD-O      core design optimization
CFR       code of federal regulation
CHF       critical heat flux
CMFD      coarse mesh finite difference
CR        control rod
CRAM      Chebyshev rational approximation method
CTF       COBRA-TF
CWO       core wide oxidation
DNB       departure from nuclear boiling
ECC       emergency core cooling
ECCS      emergency core cooling system
ECR       equivalent cladding reacted
ECRR      ECR ratio
FP        fuel performance
FTE       full-time-equivalent
FY        fiscal year
GEH       General Electric-Hitachi
HE-LL     high energy-low leakage
HPC       high performance computing
IAI       industry application 1
IEM       integrated evaluation model
INL       Idaho National Laboratory
LB-LOCA   large break LOCA
LOCA      Loss of coolant accident
LOTUS     LOCA analysis toolkit for the US
LWR       light water reactor
LWRS  Light Water Reactor Sustainability
MLO   maximum local oxidation
MOC   method of characteristics
MOOSE Multi-Physics Object-Oriented Simulation Environment
MRTAU Multi- Reactor Transmutation Analysis Utility
NEM   nodal expansion method
NPP   nuclear power plant
NRC   Nuclear Regulatory Commission
ODE   ordinary differential equation
PDE   partial differential equation
PCT   peak clad temperature
PCTR  PCT ratio
PWR   pressurized water reactor
RA    risk assessment
RELAP5 Reactor Excursion and Leak Analysis Program 5
RELAP-7 Reactor Excursion and Leak Analysis Program 7
R&D   research and development
RISMC risk informed safety margin characterization
ROM   reduced order model
SA    simulated annealing
SA    system analysis
SPH   spherical harmonics
TH    thermal hydraulics
TRISO tristructural-isotropic
VERA-CS VERA core simulator
The Nuclear Regulatory Commission (NRC) is considering a rulemaking change that would revise the requirements in 10 CFR 50.46. In the proposed new rulemaking, designated as 10 CFR 50.46(c), the NRC proposed a fuel performance-based equivalent cladding reacted (ECR) criterion as a function of cladding hydrogen content before the accident (pre-transient) in order to include the effects of higher burnup on cladding performance as well as to address other technical issues. The pre-transient cladding hydrogen content, in turn, is a function of the fuel burnup and cladding materials. The proposed rule would apply to a light water reactor and to all cladding types. The key points of the new rule are as follows:

- Cladding performance cannot be evaluated in isolation. Cladding performance and ECCS performance need to be considered in a coupled way which examines the interactions across the disciplines involved.
- Models for cladding performance even within the design basis will need to be updated for regulatory purposes.
- Effort needs to be expended in searching regulatory issue space for the limiting case (“ECCS performance must be demonstrated for a range of postulated loss-of-coolant accidents of different sizes, locations, and other properties, sufficient to provide assurance that the most severe postulated loss-of-coolant accidents have been identified. ECCS performance must be demonstrated for the accident, and the post-accident recovery and recirculation period”).

A characteristic of the proposed new rulemaking, as illustrated in Figure 1, imposes more restrictive and fuel rod-dependent cladding embrittlement criteria. Therefore, a thorough characterization of the reactor core is required in large break LOCA (LB-LOCA) analyses in order to identify the limiting case and limiting rods.

![Figure 1. Analytical Generic Limit Proposed by the NRC for Existing Fuel, ECR & PCT versus Hydrogen Content. [1]](image-url)
The final rule is expected to be issued in 2016. The rule implementation process is expected to take 5-7 years following the rule effective date. A loss of operational margin may result due to the more restrictive cladding embrittlement criteria. Initial and future compliance with the rule may significantly increase vendor workload and licensee costs as a spectrum of fuel rod initial burnup states may need to be analyzed to demonstrate compliance.

The total costs for the industry to accommodate the new rule can be in excess of $500 million. If plants have to operate at more restrictive conditions than currently allowed, the indirect cost could be even larger. Consequently, there will be an increased focus on licensee decision making related to LOCA analysis to minimize cost and impact, and to manage margin.

In 2015, as part of the DOE Light Water Reactor Sustainability Program (LWRS), Idaho National Laboratory (INL) initiated a program to develop analytical capabilities to support the industry in the transition to the new rule. One of these programs is the Industry Application 1 (IA1) within the Risk-Informed Safety Margin Characterization (RISMC) Pathway of LWRS. [2]

The general idea behind the initiative is the development of an Integrated Evaluation Model (IEM). The motivation is to revisit how uncertainties are propagated across the stream of physical disciplines and data involved, as well as how risks are evaluated in a LOCA safety analysis as regulated under 10 CFR 50.46c. The use of an integrated approach in managing the data stream is probably the most important aspect of what is proposed here. This also is well suited with current trends in industry to enhance automation and develop integrated databases across their organizations. This IEM is called LOTUS which stands for LOCA Toolkit for US, and it represents the LWRS Program’s response to the stated problem.

![Figure 2. Schematic Illustration of LOTUS.](image)
The focus of LOTUS is to establish the automation interfaces among the five disciplines as depicted in Figure 2. These five disciplines include: 1) Core Design Automation which focuses automating the cross section generation, core design and power maneuvering process, 2) Fuel Performance which focuses on automating the interface between core design and fuel performance calculations and the interface between fuel performance and system analysis, 3) System Analysis which focuses on automating the process required to setup large number of system analysis codes runs needed to facilitate RISMC applications on LOCA, 4) Uncertainty Quantification and Risk Assessment which focuses on establishing the interfaces to enable combined deterministic and probabilistic analysis, and 5) Core Design Optimization which focuses on developing core design optimization tool that can perform in-core and out-of-core design optimization.

LOTUS utilizes existing computer codes as well as advanced computer codes still being developed under various DOE programs to provide feedback and guide development of advanced tools. Regardless of the specific codes used to model the physics involved, the methodology discussed here is a paradigm shift in managing the uncertainties and assessing risks. The primary characteristic of LOTUS is to be an integrated multiphysics tool. This is a model in sharp contrast with the “operator split” or “divide-and-conquer” approach currently adopted in the industry, where every physics is resolved independently and coupling is addressed by complex interface procedures. There are significant assumptions and engineering judgment in setting up these procedures which make the propagation of uncertainties across the disciplines complex, prone to errors, and more importantly, current methods retain analytical margin which cannot be exploited.

The value proposition of LOTUS for industry stakeholders can be summarized in the following objectives:

- Provide quantitative estimates of design or operational margin loss or gain associated with various combinations of changes in LOCA analysis inputs.
- Allow/inform marketing strategies related to LOCA analysis by better informing licensees in their decision process.
- Provide LOCA inputs related studies in response to customer inquiries and requests.
- Respond to LOCA-related regulatory inquiries and requests for additional information.

Currently there are no nuclear plant owner-operators in the US that performs LOCA analysis for determining compliance with 10 CFR 50.46. In the US, Analysis of Records (AORs) are generated by nuclear vendors under contract by the plant operators. The vendor is responsible of the development of code and methods while seeking generic approval of the methodology over a target class of plants. The vendor then performs the plant specific analysis for the licensee to demonstrate compliance with the 10 CFR 50.46 criteria. The plant operator manages the analysis inputs and maintains the AORs. The vendor is responsible of managing the analysis process and assessing impact of input errors which may be found after the AOR is in place.

A limited number of owner-operators perform LOCA analysis for other purposes, such as pipe break mass and energy release or training simulator validation. For an owner-operator the LOTUS methodology and tool has two distinct types of potential applications. The more likely
type of potential applications is for LOCA analysis related work contracted to the fuel vendor,
which could include the following potential uses:

- Obtain quantitative estimates of design or operational margin loss or gain associated with
  various combinations of changes in LOCA analysis inputs.

- Obtain quantitative estimates of impact on the LOCA analysis figures-of-merit due to
  changes in LOCA analysis inputs (including reporting of LOCA analysis ΔPCT and ΔECR
  due to LOCA analysis input changes that are required by 10 CFR 50.46).

Another possible type of potential application is to use the LOTUS methodology and tools
as an independent owner-operator LOCA analysis capability, especially LOTUS requires
minimum infrastructure and training for its usage. This capability could be used to perform
vendor-independent LOCA scoping or audit calculations that would facilitate decision making
related to the impact of plant and fuel design changes, as well as provide an enhanced vendor
oversight capability. An owner-operator could develop this capability with in-house staff or by
outsourcing to an engineering services or consulting entity.

Another important driver of developing LOTUS is the elimination of issues associated
with the so-called Wilks’ approach [3] (variability in the estimator, i.e. risk of under-prediction
of or over-prediction of figures of merit, lack of knowledge in what’s truly limiting in the design,
incapacity to perform sensitivity studies, impact assessment etc.). Despite its widespread
adoption by the industry (AREVA, GEH and Westinghouse), the use of small sample sizes to
infer statement of compliance to the 10 CFR 50.46 rule, has been a cause of unrealized
operational margin in today’s best-estimate plus uncertainty methods. Moreover, the debate on
the proper interpretation of the Wilks’ theorem in the context of safety analyses is not fully
resolved yet more than a decade after its introduction in the frame of safety analyses in the
nuclear industry. This represents both a regulatory and applicant risk in rolling out new methods.

The new rule added another layer of complexity for the demonstration of compliance.
Under the current rule PCT, Maximum Local Oxidation (MLO) and Core Wide Oxidation limits
are set to specific value (2200 F, 17% and 1% respectively). Using Wilks compliance is easily
demonstrated by ranking the corresponding values obtained from the simulations in the sample
and ensuring the rank representing the 95/95 estimate from a small sample is below those limits.
Considering there are three outcomes (PCT, MLO and CWO), the highest ranked set from a
sample of 124 can be chosen.

With new rule the limit is a curve, more specifically both PCT and MLO (maximum
Equivalent Clad Reacted (ECR) in this case) limits are functions of cladding hydrogen content
which varies from rod to rod in the core. Applying Wilks’ method would require to define new
figure of merits that synthetize this relationship. Additionally, if the analyst is ultimately
interested in tracking the margin in each core region, that would not be possible unless a much
larger sample size is used. With LOTUS, the answer is to move toward full Monte Carlo
simulations when it comes to managing uncertainties. It has to be acknowledged that the sample
size needed to reduce the confidence interval on the estimate (standard error) to the magnitude
desired may require sample sizes in excess of 1,000-10,000 cases. However the benefit is that
full Monte Carlo simulations enable to assess the impact of input parameter changes to
distribution and determine the significance of the change.
2. TECHNICAL APPROACH

The first step in obtaining the desired technical capability to perform the type of analyses that address the challenges presented in Section 1 is to revisit how uncertainties are propagated across the stream of physical disciplines involved. Regardless the specific codes used to model the physics involved, the methodology discussed here is really a different strategy in managing the uncertainties.

As stated in Section 1, the primary objective of LOTUS is to be an integrated multiphysics tool. In the LOTUS framework uncertainties are propagated directly from all the uncertain design and model parameters. The interactions between the various model parameters are directly solved within the LOTUS framework.

This interaction not only facilitates the automation of the process, but it is also mathematically more robust because the advanced procedure considered to propagate uncertainties and/or perform global sensitivity and risk studies requires inputs sampled to be independent. This requirement is hard to achieve following the traditional “divide-and-conquer” approach.

![LOTUS Data Stream Diagram]

Figure 3. LOTUS Data Stream.

Conventional methods are strongly “code-oriented.” The analyst has to be familiar with the details of the codes utilized, in particular with respect to their input and output structures. This represents a significant barrier for widespread use beside the small pool of experts within the specific organization or even groups within the organization that develops such codes. It becomes apparent how difficult is to make changes and accelerate progress under such paradigm,
especially in heavily regulated environment where even a minor line changes in a code carries a heavy cost of bookkeeping and regulatory actions.

Our vision is to move toward to a “plug and play” or “task oriented” approach where the codes are simply modules ‘under the hood’ that provides the input-output relationship for a specific discipline. The focus shifts on managing the data stream at a system level, as depicted in Figure 3. LOTUS is essentially a workflow engine with capability to drive physics simulators, model complex systems and provide risk assessment.

As a multi-physics analytical framework, LOTUS is not intended to replace licensing Analysis of Records (AORs), but rather to replace or aid the “engineering judgment” which is typically applied in the management and maintenance of those AORs. The goal is an analytical and computational device that can represent a power plant realistically with all the uncertainties included and that considers all physical disciplines involved in an integrated fashion.

A “plug-and-play” approach will enable plant owners and vendors to consider and further customize the LOTUS framework for use within their established codes and methods. Therefore, it could potentially become the engine for license-grade methodologies. In other words, it is possible that LOTUS technology could be advanced in the future to a level of fidelity and maturity that it could be used for some licensing or regulatory situations. An example would be the reporting of LOCA analysis \( \Delta PCT \) and \( \Delta ECR \) due to LOCA analysis input changes that are required by 10 CFR 50.46c.

As a first step, the owner/operator may use LOTUS to “characterize” the core designed for operation. Figure 4 illustrates this process, where LOTUS maps an envelope of maximum ECR as a function of cycle exposure. This allows the operator to have a realistic assessment of an operating core, and conceivably be more prepared for a quick response re-analysis in case a problem might occur.

![Figure 4. Margin Characterization Schematic.](image-url)
The characterization of a reference core with LOTUS is intended to simplify the existing reload analysis process, without replacing the existing licensing process. In principle, a reload engineer that has trained with the LOTUS tools to analyze a given core design can re-analyze such reference design in much faster time than using a traditional reload design analysis process.

The ultimate goal is then to incorporate optimization schemes in LOTUS that can quickly reshape a desired parameter envelope (for example ECR) as an optimization feature of a core design process. This step will require additional changes to today’s design process, in order to incorporate LOCA analysis as an integrated element of the reload analysis process.

3. DESCRIPTION OF COMPUTER CODES USED BY LOTUS

3.1 PHISICS

PHISICS is a neutronics code system in development at INL. [4] The different modules for PHISICS are a nodal and semi-structured spherical harmonics–based transport core solver [Intelligent Nodal and Semi-structured Treatment for Advanced Neutron Transport (INSTANT)] [5] for steady-state and time-dependent problems, a depletion module [Multi-Reactor Transmutation Analysis Utility (MRTAU)], [6] and a cross-section mixer-interpolator (MIXER) module. [7] Each different module of PHISICS contains a kernel (module) that solves a basic problem. A local driver is assigned to each kernel that is able to run it in stand-alone mode. Communication between the kernels is managed by the use of global data types that hold global information (cross-section data, mesh, fluxes, etc.) that are needed by more than one kernel to perform complex calculations involving different kernels. Global drivers solving a complex problem calling different kernels can be developed easily with this flexible software structure. The PHISICS code is still in development to extend its capabilities.

The transport core solver INSTANT is the key kernel of the PHISICS framework. INSTANT is parallelized and is designed to take full advantage of medium to large clusters (10 to 1000 processors). It is based on the second-order formulation of the transport equation discretized in angle by spherical harmonics while in space it uses orthonormal polynomials of an arbitrary order. In addition to steady-state solutions, INSTANT is able to solve time-dependent problems. For that, a scheme based on a second-order backward Euler scheme with explicit delayed neutron treatment has been implemented as a new module for the PHISICS suite.

MRTAU is a generic depletion code developed at INL. [6] In addition to core depletion, the code can be utilized for stand-alone decay heat calculations. It tracks the time evolution of the isotopic concentration of a given material accounting for nuclear reactions occurring in the presence of neutron flux and also due to natural decay (Bateman equation). The code uses a Taylor series expansion–based algorithm at arbitrary order and the Chebyshev Rational Approximation Method (CRAM) for computation of the exponential matrix.

The MIXER module does all the cross-section handling for the different kernels. MIXER can handle macroscopic, microscopic, and “mixed” cross sections. A macroscopic cross-section library contains macroscopic cross sections for each type of material used in the calculation.
(fuel, reflector, etc.) tabulated for the state parameters (temperature, burnup, CR position, etc.). MIXER interpolates these cross sections at the requested state parameters, and no limits in tabulation dimensions or neutron energy groups exist. A microscopic or mixed cross-section library contains the tabulated cross sections for each isotope considered in the calculation. MIXER reads a description containing a list of isotopes and corresponding densities for each material and interpolates the microscopic cross sections at the requested state parameters. Macroscopic cross sections for each material are generated with the corresponding number densities. With this capability, mixed macroscopic and microscopic cross sections are also possible. For example, it is possible to provide macroscopic absorption cross sections without xenon for a material and the microscopic xenon absorption cross section together with a xenon density. MIXER will calculate the xenon absorption contribution and add it to the macroscopic cross section. MIXER can read different cross-section library formats. Among them is an original simple XML-based format, but also AMPX, ISOTXS, and ECCO library formats that allow cross-section libraries to be prepared with SCALE, ERANOS, or MC2. More library types are planned to be supported in the future.

The PHISICS code is currently being used as the core design tool in LOTUS. Only the assembly power is available in PHISICS. The lack of pin power capability could limit its applications in LOTUS.

### 3.2 NESTLE

NESTLE [8] is a few-group multi-dimensional nodal core simulator. It employs the nodal expansion method (NEM) to solve the few-group neutron diffusion equations. The NESTLE reactor core simulator was developed originally in the late 1980s at North Carolina State University and has been used widely over the last twenty years. NESTLE utilizes the nodal expansion method for eigenvalue, adjoint, fixed source steady-state and transient problems. A collaboration among the University of Tennessee, Oak Ridge National Laboratory, and North Carolina State University during the last five years has led to a new and improved version of NESTLE written in modern Fortran and developed with modern software engineering practices. New features include a simplified input format, a drift-flux model for high slip two-phase thermal hydraulics, advanced depletion and isotope tracking using ORIGEN, output files compatible with VISIT visualization software, and compatibility with SCALE, SERPENT, and CASMO lattice physics. The new features have expanded NESTLE’s versatility from large pressurized water reactors to new core models including boiling water reactors, small modular reactors, and fluoride salt cooled high temperature reactors. NESTLE has unique capabilities like advanced isotope tracking.

NESTLE is a mature code and will be explored as an alternative baseline core design tool in FY-2017.

### 3.3 MAMMOTH

MAMMOTH [9] is the reactor physics application for the MOOSE framework and combines the capabilities of the Rattlesnake solver (steady state and transient neutron transport), BISON (fuels performance) and RELAP-7 (thermal/hydraulics). MAMMOTH contains cross section interpolation and depletion capabilities required for cycle analysis with Rattlesnake,
using temperature data provided by BISON. Individually, these packages provide little to no advantage over existing methods, but combined within MAMMOTH provide a powerful and tightly coupled multi-physics capability not available elsewhere. This provides the ability to better quantify multiple performance aspects of the core design concept under normal and off-normal conditions. MAMMOTH can prepare cross section libraries from DRAGON-5 and Serpent lattice physics calculations. In addition, MAMMOTH includes an SPH equivalence methodology, which enables the preservation of the lattice physics reaction rates and, thus, provide highly accurate calculations. MAMMOTH does not currently support pin power reconstruction but most of the LWR models in place are pin-cell models, which directly resolve accurate pin powers.

MAMMOTH is an advanced core design code still being developed at INL. Certain features required for LWR analysis such as core shuffling and fuel burnup calculations are not available yet and may be developed in FY-2016 and FY-2017.

3.4 VERA-CS

VERA-CS [10] includes coupled neutronics, thermal-hydraulics, and fuel temperature components with an isotopic depletion capability. The neutronics capability employed is based on MPACT, [11] a three-dimensional (3-D) whole core transport code. The thermal-hydraulics and fuel temperature models are provided by the COBRA-TF (CTF) subchannel code. [12] The isotopic depletion is performed using the ORIGEN code system.

3.4.1 MPACT

MPACT [11] is a 3-D whole core transport code that is capable of generating subpin level power distributions. This is accomplished by solving an integral form of the Boltzmann transport equation for the heterogeneous reactor problem in which the detailed geometrical configuration of fuel components, such as the pellet and cladding, are explicitly retained. The cross section data needed for the neutron transport calculation are obtained directly from a multigroup cross section library, which has traditionally been used by lattice physics codes to generate few-group homogenized cross sections for nodal core simulators. Hence, MPACT involves neither a priori homogenization nor group condensation for the full core spatial solution.

The integral transport solution is obtained using the method of characteristics (MOC), and employs discrete ray tracing within each fuel pin. MPACT provides a 3-D MOC solution; however, for practical reactor applications, the direct application of MOC to 3-D core configuration requires considerable amounts of memory and computing time associated with the large number of rays. Therefore, an alternative approximate 3-D solution method is implemented in MPACT for practical full core calculations, based on a “2D/1D” method in which MOC solutions are performed for each radial plane and the axial solution is performed using a lower-order one-dimensional (1-D) diffusion or SP3 approximation. The core is divided into several planes, each on the order of 5-10 cm thick, and the planar solution is obtained for each plane using 2D MOC. The axial solution is obtained for each pin, and the planar and axial problems are coupled through a transverse leakage. The use of a lower order 1-D solution, which is most often the nodal expansion method (NEM) with the diffusion or P3 approximation, is justified by the fact that most heterogeneity in the core occurs in the radial direction rather than the axial
direction. Alternatively, a full 3D MOC solution can be performed, if the computational resources are available.

The Coarse Mesh Finite Difference (CMFD) acceleration method, which was originally introduced to improve the efficiency of the nodal diffusion method, is used in MPACT for the acceleration of the whole core transport calculation. The basic mesh in the CMFD formulation is a pin cell, which is much coarser than the flat source regions defined for MOC calculations (typically there are on the order of fifty (50) flat source regions in each fuel pin). The concept of dynamic homogenization of group constants for the pin cell is the basis for the effectiveness of the CMFD formulation to accelerate whole core transport calculations. The intra-cell flux distribution determined from the MOC calculation is used to generate the homogenized cell constants, while the MOC cell surface-averaged currents are used to determine the radial nodal coupling coefficients. The equivalence formalism makes it possible to generate the same transport solution with CMFD as the one obtained with the MOC calculation. In addition to the acceleration aspect of the CMFD formulation, it provides the framework for the 3-D calculation in which the global 3-D neutron balance is performed through the use of the MOC generated cell constants, radial coupling coefficients, and the NEM generated axial coupling coefficients.

In the simulation of depletion, MPACT can call the ORIGEN code, which is included in the SCALE package. However, MPACT has its own internal depletion model, which is based closely on ORIGEN, with a reduced isotope library and number of isotopes. The internal depletion model has been used for this study.

3.4.2 COBRA-TF

COBRA-TF (Coolant Boiling in Rod Arrays – Two Fluid) [12] is a transient subchannel code based on two-fluid formulation that separates the conservation equations of mass, energy, and momentum to three fields of vapor, continuous liquid, and entrained liquid droplets. The conservation equations for the three fields and for heat transfer from and within fuel rods are solved using a semi-implicit and finite-difference numerical scheme, using closure equations to account for inter-phase mass and heat transfer and drag, mechanical losses, inter-channel mixing, and fluid properties. The code is applicable to flow and heat transfer regimes beyond CHF, and is capable of calculating reverse flow, counter flow and crossflow with either three-dimensional (3D) Cartesian or subchannel coordinates for TH or heat transfer solutions. It allows for full 3D LWR core modeling and has been used extensively for LWR Loss-Of-Coolant Accident (LOCA) and non-LOCA analyses including the DNB analysis.

The COBRA-TF (CTF) code was originally developed by the Pacific Northwest Laboratory and has been updated over several decades by several organizations. CTF is being further improved as part of the VERA multi-physics software package, including:

- Improvements to user-friendliness of the code through creation of a PWR preprocessor utility,
- Code maintenance, including source version tracking, bug fixes, and transition to modern Fortran,
- Incorporation of an automated build and testing system using CMake/CTest/Tribits,
- Addition of new code outputs for better data accessibility and simulation visualization,
• Extensive source code optimizations and full parallelization of the code, enabling fast simulation of full core subchannel models,
• Improvements to closure models, including Thom boiling heat transfer model and Yao-Hochreiter-Leech grid-heat-transfer enhancement model, and Tong factor for the W-3 CHF correlation,
• Addition of consistent set of steam tables from IAPWS-97 standard,
• Application of extensive automated code regression test suite to prevent code regression during development activities,
• Code validation study with experimental data.

In a steady-state or transient CTF simulation, subchannel data, such as flow rate, temperature, enthalpy, and pressure and fuel rod temperatures are projected onto a user-specified or pre-processor generated mesh and written to files in a format suitable for visualization. The freely available Paraview software is used for visualizing three-dimensional data resulting from large full core models and calculations.

The steady-state analysis capability for VERA-CS is available. However VERA-CS is computationally prohibitive and requires HPCs with several thousand cores. Therefore, it will be adapted in LOTUS in FY-2017 as a benchmark tool to check the final designs obtained from the baseline tools.

3.5 FRAPCON/FRAPTRAN

FRAPCON [13] is a computer code that calculates the steady-state response of light-water reactor fuel rods. 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. The code contains necessary material properties, water properties, and heat-transfer correlations. Other input parameters to the RELAP5 model required from FRAPCON include the gap closure and cladding roughness. The internal pressure is required from FRAPCON calculations in order for RELAP5 to perform clad ballooning and rupture calculations. The FRAPCON results are needed to initialize the fuel heat structure models as a part of calculating the steady-state solution that initializes the LOCA transient simulations.

The Fuel Rod Analysis Program Transient (FRAPTRAN) [14] is a FORTRAN language computer code that calculates the transient performance of light-water reactor fuel rods during reactor transients and hypothetical accidents such as loss-of-coolant accidents, anticipated transients without scram, and reactivity-initiated accidents. FRAPTRAN calculates the temperature and deformation history of a fuel rod as a function of time-dependent fuel rod power and coolant boundary conditions. Although FRAPTRAN can be used in “standalone” mode, it is often used in conjunction with, or with input from, other codes. 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.
FRAPCON/FRAPTRAN codes are mature codes and will be used as the baseline fuel performance simulations tools in LOTUS.

3.6 BISON

BISON [15] is a finite element-based nuclear fuel performance code applicable to a variety of fuel forms including light water reactor fuel rods, TRISO particle fuel, and metallic rod and plate fuel. It solves the fully-coupled equations of thermo-mechanics and species diffusion, for either 1D spherical, 2D axisymmetric or 3D geometries. Fuel models are included to describe temperature and burnup dependent thermal properties, fission product swelling, densification, thermal and irradiation creep, fracture, and fission gas production and release. Plasticity, irradiation growth, and thermal and irradiation creep models are implemented for clad materials. Models are also available to simulate gap heat transfer, mechanical contact, and the evolution of the gap/plenum pressure with plenum volume, gas temperature, and fission gas addition. BISON has been coupled to the mesoscale fuel performance code MARMOT, demonstrating fully-coupled multiscale fuel performance capability. BISON is based on the MOOSE framework and can therefore efficiently solve problems using standard workstations or very large high-performance computers. BISON is currently being validated against a wide variety of integral light water reactor fuel rod experiments.

BISON is an advanced fuel performance code being developed at INL and offers distinctive advantages over FRAPCON/FRAPTRAN such as 3D simulation capability, etc. However, for LWR LOCA analyses, certain models such as cladding hydrogen uptake, cladding oxidation, etc. are not yet fully developed. As those models become well developed, BISON will be incorporated into LOTUS starting in FY-2017.

3.7 RELAP5-3D

The RELAP5-3D [16] code has been developed for best-estimate transient simulation of light water reactor coolant systems during postulated accidents. Specific applications of the code have included simulations of transients in light water reactor (LWR) systems such as loss of coolant, anticipated transients without scram (ATWS), and operational transients such as loss of feedwater, loss of offsite power, station blackout, and turbine trip. RELAP5-3D, the latest in the series of RELAP5 codes, is a highly generic code that, in addition to calculating the behavior of a reactor coolant system during a transient, can be used for simulation of a wide variety of hydraulic and thermal transients in both nuclear and nonnuclear systems involving mixtures of vapor, liquid, non-condensable gases, and nonvolatile solute.

RELAP5-3D is suitable for the analysis of all transients and postulated accidents in LWR systems, including both large- and small-break loss-of-coolant accidents (LOCAs) as well as the full range of operational and fusion reactor transient applications. Additional capabilities include space reactor simulations, gas cooled reactor applications, fast breeder reactor modeling, and cardiovascular blood flow simulations.

The RELAP5-3D© code is based on a non-homogeneous and non-equilibrium model for the two-phase system that is solved by a fast, partially implicit numerical scheme to permit economical calculation of system transients. The objective of the RELAP5-3D development
effort from the outset was to produce a code that included important first-order effects necessary for accurate prediction of system transients but that was sufficiently simple and cost effective so that parametric or sensitivity studies were possible.

The code includes many generic component models from which general systems can be simulated. The component models include pumps, valves, pipes, heat releasing or absorbing structures, reactor kinetics, electric heaters, jet pumps, turbines, compressors, separators, annuli, pressurizers, feedwater heaters, ECC mixers, accumulators, and control system components. In addition, special process models are included for effects such as form loss, flow at an abrupt area change, branching, choked flow, boron tracking, and non-condensable gas transport.

The system mathematical models are coupled into an efficient code structure. The code includes extensive input checking capability to help the user discover input errors and inconsistencies. Also included are free-format input, restart, renodalization, and variable output edit features. These user conveniences were developed in recognition that generally the major cost associated with the use of a system transient code is in the engineering labor and time involved in accumulating system data and developing system models, while the computer cost associated with generation of the final result is usually small.

RELAP5-3D is a mature code for LOCA analysis and will be the initial working engine and baseline tool for LOTUS.

3.8 RELAP-7

The RELAP-7 [17] (Reactor Excursion and Leak Analysis Program) code is the next generation nuclear reactor system safety analysis code being developed at Idaho National Laboratory (INL). The code is based on the INL’s modern scientific software development framework MOOSE (Multi-Physics Object Oriented Simulation Environment). The overall design goal of RELAP-7 is to take advantage of the previous thirty years of advancements in computer architecture, software design, numerical integration methods, and physical models. The end result will be a reactor systems analysis capability that retains and improves upon RELAP5-3D’ capability and extends the analysis capability for all reactor system simulation scenarios.

The RELAP-7 project, which began in Fiscal Year 2012, will become the main reactor systems simulation toolkit for LWRS (Light Water Reactor Sustainability) program’s RISMC (Risk Informed Safety Margin Characterization) effort and the next generation tool in the RELAP reactor safety/systems analysis application series. The key to the success of RELAP-7 is the simultaneous advancement of physical models, numerical methods, and software design while maintaining a solid user perspective. Physical models include both PDEs (Partial Differential Equations) and ODEs (Ordinary Differential Equations) and experimental based closure models. RELAP-7 will utilize well-posed governing equations for two-phase flow, which can be strictly verified in a modern verification and validation effort. Closure models used in RELAP5 and other newly developed models will be reviewed and selected to reflect the progress made during the past three decades and provide a basis for the closure relations that will be required in RELAP-7. RELAP-7 uses modern numerical methods, which allow implicit time integration, second-order schemes in both time and space, and strongly coupled multi-physics.
RELAP-7’s analysis capabilities need further development to be able to be used to perform LOCA analysis. Based on the current development schedule for RELAP-7, it will be ready to be incorporated into LOTUS in FY-2018 to perform LOCA analysis.

3.9 RAVEN

RAVEN [18] is a software framework able to perform parametric and stochastic analysis based on the response of complex system codes. The initial development was aimed at providing dynamic risk analysis capabilities to the thermohydraulic code RELAP-7, currently under development at Idaho National Laboratory (INL). Although the initial goal has been fully accomplished, RAVEN is now a multi-purpose stochastic and uncertainty quantification platform, capable of communicating with any system code. In fact, the provided Application Programming Interfaces (APIs) allow RAVEN to interact with any code as long as all the parameters that need to be perturbed are accessible by input files or via python interfaces. RAVEN is capable of investigating system response and explore input space using various sampling schemes such as Monte Carlo, grid, or Latin hypercube. However, RAVEN’s strength lies in its system feature discovery capabilities such as: constructing limit surfaces, separating regions of the input space leading to system failure, and using dynamic supervised learning techniques.

RAVEN will be used to perform risk analysis for the baseline simulation tools as well as for the advanced simulation tools.

3.10 LWROPT

A new computer software for performing LWR (with the emphasis of PWR) in-core and out-of-core fuel cycle optimization for multiple cycles simultaneously may be developed within the LOTUS framework. The computer code is called LWROPT. Simulated annealing (SA) is used to optimize the new fuel inventory and loading pattern for each cycle considered. 3-D core simulators such as PHISICS and NESTLE are used to perform loading pattern calculations in conjunction with simulated annealing. LWROPT will have features including: 1) User controlled depletion schedule; 2) Spent fuel pool simulation which allows fuel assemblies to be reinserted into the reactor core; 3) Multi-cycle optimization capability; 4) User defined coastdown option; 5) Automated equilibrium cycle design; 6) Loading pattern design optimization using simulated annealing.

LWROPT can give utilities the power to perform their own fuel design analyses. These include: design of the core loading pattern and control rod pattern for future cycles, assess a fuel vendor proposed core design to confirm that it meets requirements or to achieve a more efficient design, perform fuel bid evaluations to compare fuel design proposals from multiple fuel vendors using the same point of reference, explore various fuel designs with respect to batch feed size (impact on cycle length, thermal margins), the ability to quickly explore a wide range of core designs that can lead to a better core design still meeting safety margins.

LWROPT does not yet exist. The development effort is envisioned according to the plan presented in the next section.
4. PROJECT PLANNED SCHEDULE

The LOTUS project will be developed in two phases. First, for fiscal years 2016-17 we will demonstrate LOTUS-B, using ‘Baseline’ (already existing) RISMC tools and methods to demonstrate the first four elements (1-4) of Figure 5, core design automation (CD-A), fuels/clad performance (FP), systems analysis (SA), and UQ and risk assessment (RA) methods. Second, for fiscal years 2017-19, we will demonstrate all five elements (1-5) of LOTUS-A of Figure 5, which will include ‘Advanced’ (in development by LWRS and other DOE R&D Programs) RISMC tools and methods, including core design optimization (CD-O) advanced schemes.

4.1 Phase I – LOTUS-B (Baseline)

For the first two years, four elements (1 through 4 in Figure 5) of the LOTUS-B toolkit are exercised. Each element implements a set of existing, well established code(s) into the LOTUS-B toolkit, as illustrated in Figure 5 by (B). A set of all activities to be executed within this timeline is outlined in Table 1.

4.2 Phase II – LOTUS-A (Advanced)

In conjunction with the Baseline development, for a period of about three years, the advanced phase of the LOTUS project will be executed (fiscal years 2017-19). The duration and timeline associated with the LOTUS-A phase is in part dependent on the execution and lessons learned of the Baseline phase, and availability and maturity of the advanced tools in development today. An example of tools and methods to be implemented during the advanced phase is shown in Figure 5 by the (A) symbol. Also, a set of all activities to be executed during Phase II is outlined in Table 1.

Figure 5. Schematic Illustration of LOTUS-A and LOTUS-B.
Table 1. LOTUS-A/B Timeline of Activities and Resources for each Area of Development.

<table>
<thead>
<tr>
<th>Technical Areas</th>
<th>Phase I: LOTUS-B</th>
<th>Phase II: LOTUS-A</th>
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</thead>
<tbody>
<tr>
<td>Core Design</td>
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<td>Automation (CD-A)</td>
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<td>Fuel/Clad</td>
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<td>Performance (FP)</td>
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<td>Systems</td>
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<td>Analysis (SA)</td>
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<tr>
<td>Uncertainty Quantification and Risk Assessment (RA)</td>
<td>Core Design Optimization (CD-O)</td>
<td>Overall LOTUS Project</td>
</tr>
<tr>
<td>--------------------------------------------------</td>
<td>---------------------------------</td>
<td>----------------------</td>
</tr>
<tr>
<td>Enhance BEPU analysis capability to expand uncertain parameter table 0.2 FTE</td>
<td>Assess the LOTUS framework (Software and data structure) 0.1 FTE</td>
<td>Establish the LOTUS framework (Software and data structure) 0.1 FTE</td>
</tr>
<tr>
<td>Demonstrate fuel performance surrogate models with RAVEN 0.3 FTE</td>
<td>Develop the core design optimization algorithm for LWROPT 0.5 FTE</td>
<td>Refine LOTUS framework to improve the automation process 0.1 FTE</td>
</tr>
<tr>
<td>Demonstrate UQ using reduced order methods (ROM) and limit surfaces with RAVEN 0.3 FTE</td>
<td>Implement core design optimization algorithm into LOTUS 0.3 FTE</td>
<td>Integration of advanced simulation tools into the LOTUS framework 0.4 FTE</td>
</tr>
<tr>
<td>Develop dynamic PRA model for LOCA analysis 0.4 FTE</td>
<td>Demonstrate combined PRA and deterministic analysis for LOCA 0.3 FTE</td>
<td>Demonstrate optimized core design with LWROPT 0.5 FTE</td>
</tr>
<tr>
<td>Demonstrate combined PRA and deterministic analysis for LOCA 0.3 FTE</td>
<td></td>
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</tbody>
</table>

| TOTAL | 3.7 FTEs | 3.1 FTEs | 1.6 FTEs | 3.0 FTEs | 3.0 FTEs |

![Fiscal Year Resources (full-time-equivalent)](image)

Figure 6. Fiscal Year Estimated Resources for LOTUS-A/B.
4.3 Planned Resources

The anticipated time for completion of LOTUS-B and LOTUS-A are two years and three years, respectively. The time for completion of the LOTUS tools may however vary depending on actual funding levels per fiscal year. The resources per task shown in Table 1 are estimates at this time, and may vary as well for the same reasons.

The resources required to successfully execute the planned work shown above are: 3.7 FTEs for FY-2016; 4.7 FTEs for FY-2017; 3 FTEs for FY-2018; and 3 FTEs for FY-2019. The planned resources are illustrated in Figure 6.

5. ANTICAPTED OUTCOME

The intrinsic value of a successful R&D in this area is expected to be significant. LOTUS has the potential of becoming the toolkit of choice by industry stakeholders to address the challenges imposed by the 10 CFR 50.46c proposed rulemaking, by relying on a more rigorous mathematical approach to address the important issue of uncertainties when dealing with safety analyses.

Once LOTUS achieves its objectives, it can potentially outweigh some of the costs associated with the proposed rule rollout, therefore keeping the US LWR fleet competitive with other sources of energy. A more informed analyst with respect to actual margins available in an operating plant can potentially reduce extensive (and costly) iterations between licensee and regulators when dealing with rule compliance issues. Ultimately more information will yield a higher degree of safety and improving economics.

For FY-2016, a notable outcome milestone for the Idaho National Laboratory, as one of its performance measures, has been planned to demonstrate the capabilities described in this paper. The narrative of the Notable Outcome 1.1.C milestone is as follows:

Based upon recent experiments, the NRC has proposed new peak-clad temperature and embrittlement oxidation limits that are more restrictive than the current operational limits which may impact current plant operational margin, increase plant fuel/analysis costs, limit the use of high burnup fuels, increase the complexity of analysis, decrease optional flexibility, and increase regulatory uncertainties. INL’s Light Water Reactor Sustainability Program will help industry address this issue by using the Risk-Informed Safety Margin Characterization approach to demonstrate safety margins using coupled analysis tools for a loss-of-coolant-accident (LOCA) analysis including Emergency Core Cooling System (ECCS) performance under realistic plant conditions. This risk-informed analysis will include the effects of higher burnup on cladding performance as part of the LOCA/ECCS analysis in order to evaluate risk-informed margins management strategies for a representative pressurized water reactor. The integrated coupled analysis will include elements of core physics, cladding behavior, thermal-hydraulics, and scenario-based risk analysis in order to quantify safety margin for the new peak-clad temperature and embrittlement oxidation limits.
6. REFERENCES


