GA-A29407
ORNL/LTR-2020/1657

ACCELERATED FUEL QUALIFICATION (AFQ) WORKSHOP I SUMMARY REPORT

Prepared Under
Contract DE-NE0008819
and
Contract DE-NE0008831

Presented May 31, 2019

Complied By
R. Faibish
General Atomics

DISCLAIMER

GENERAL ATOMIC PROJECT 30543
NOVEMBER 2020

GENERAL ATOMICS

TABLE OF CONTENTS

LIST OF TABLES

FOREWORD

The files contained in this report are the compilation of all materials pertaining to the first workshop on Accelerated Fuel Qualification (AFQ): AFQ Workshop I. The overall goal of the workshop was to discuss how modeling and experiments can be simultaneously exploited to markedly reduce the years of data (and associated costs) that are currently required for deployment of new nuclear fuels utilizing the new AFQ methodology.

1 BRIEF OVERVIEW

The first AFQ workshop was held on Friday, May 31, 2019, in Washington, DC, with over 30 expert participants from industry (General Atomics, Framatome, Lightbridge, TerraPower, Westinghouse), national labs (ANL, INL, LANL, ORNL), DOE-NE, NRC and academia (University of Florida and University of Tennessee). **The overall goal of the workshop was to discuss how modeling and experiments can be simultaneously exploited to markedly reduce the years of data (and associated costs) that are currently required for deployment of new nuclear fuels utilizing the new methodology of Accelerated Fuel Qualification (AFQ).** There were nine presentations given during the workshop, which included an overview presentation, five case studies, summary of relevant national lab capabilities and on-going DOE programs, as well as perspective from the NRC.

2 WORKSHOP AGENDA AND PARTICIPANTS

Table 1. Workshop Agenda

Time	Agenda Item
08:30-08:50	Welcome and introductions
08:50-09:20	AFQ Overview: what is AFQ and why is it important?
09:20-11:00	Example case studies
11:00-11:15	Break
11:15-12:30	Elements of AFQ: DOE Lab capabilities and approaches: Computational & Experimental
12:30-13:30	Lunch
13:30-14:15	NRC perspectives
14:15-15:45	Open discussion
15:45-16:00	Break
16:00-16:45	Next steps
16:45	Adjourn

Table 2. Workshop Participants

Affiliation	Name	Email
Argonne National Lab		
	Abdellatif (Latif) Yacout	yacout@anl.gov
Department of Energy		
	Janelle Eddins	janelle.eddins@nuclear.energy.gov
	Madeline Feltus	madeline.feltus@nuclear.energy.gov
	Frank Goldner	frank.goldner@nuclear.energy.gov
	David Henderson	david.henderson@nuclear.energy.gov
	Bill McCaughey	bill.mccaughey@nuclear.energy.gov
Framatome		
	Joshua Parker	josh.parker@framatome.com

Affiliation	Name	Email
General Atomics		
	Christina Back	Christina.Back@ga.com
	John Bolin	John.Bolin@ga.com
	Ron Faibish	Ron.Faibish@ga.com
Idaho National Lab		
	Steve Hayes	steven.hayes@inl.gov
	Matthew Kerr	Matthew.Kerr@inl.gov
Lightbridge Corporation		
	Jim Fornof	JFornof@Ltbridge.com
	Aaron Totemeier	Atotemeier@ltbridge.com
Los Alamos National Lab		
	David Andersson	andersson@lanl.gov
	Ken McClellan	kmcclellan@lanl.gov
	Chris Stanek	stanek@lanl.gov
Nuclear Regulatory Commission		
	Travis Boyce	travis.boyce@nrc.gov
	Paul Clifford	Paul.Clifford@nrc.gov
	Tim Drzewiecki	tim.drzewiecki@nrc.gov
	Lucas Kyriazidis	Lucas.Kyriazidis@nrc.gov
	Jeff Schmidt	paul.schmidt@nrc.gov
	Chris Van Wert	Christopher.VanWert@nrc.gov
Oak Ridge National Lab		
	Andrew Nelson	nelsonat@ornl.gov
	Kurt Terrani	terranika@ornl.gov
TerraPower		
	Pete Gaillard	pgaillard@terrapower.com
	James Vollmer	jvollmer@terrapower.com
University of Florida		
	Michael Tonks	michael.tonks@ufl.edu
University of Tennessee-Knoxville		
	Brian Wirth	bdwirth@utk.edu
Westinghouse		
	Andrew Bowman	bowmanab@westinghouse.com
	Zeses Karoutas	karoutze@westinghouse.com
	Kathryn Metzger	metzgeke@westinghouse.com

3 AFQ DEFINITION

The combination of physics-informed advanced nuclear fuel performance modeling and simulation (m&s) tools with targeted irradiation and other select experimental data that can significantly reduce the cost and number of integral irradiation tests and, ultimately, the cost and time associated with new fuel qualification.

4 HIGH-LEVEL TAKEAWAYS

4.1 Agreed-upon Status Today

1. Significant advancements in computational power and tools in the recent years have enabled the increasingly accurate prediction of material properties and behavior from basic principles through complex meso and engineering scale phenomena.
2. Experimental capabilities, such as the ORNL mini-capsule and the INL FAST irradiation vehicles, are emerging elements that can be used in a systematic AFQ methodology. Importantly, they enable a new-class of targeted experiments and complement work already occurring at the DOE-funded facilities such as ATR, HFIR, TREAT, LAMDA, and others.
3. The DOE NEAMS and AFC programs are well positioned to assist in developing and implementing AFQ. Discussion in this workshop demonstrated that we don’t have all the pieces needed to implement AFQ.
4. NRC sees additional flexibility in licensing of advanced non-LWRs when compared to LWRs, given the already well-understood process associated with the latter.
5. The NRC participants are quite willing to explore and assess applicability and usefulness of the AFQ methodology in the qualification and licensing of new fuels
6. DOE is supportive of the concept.
7. Further discussion is needed to determine whether (a) a generic approach to AFQ should be developed; (b) simultaneous development of a generic approach and specific demo projects that address new fuel needs for a specific reactor system is recommended; or (c) no generic approach can be established and AFQ can only be demonstrated via specific demo projects
8. Developing AFQ to address accident scenarios would be important.

4.2 The What’s and Why’s of AFQ

1. By exploiting advanced m&s tools to inform choice of targeted experiments and data acquisition, the AFQ methodology has the potential to reduce the high number of new nuclear integral tests that are required to qualify new fuels while maintaining the highest safety standards and requirements. All participants strongly agree that the AFQ methodology **in no way** will substitute the need for integral fuel testing.
2. The time for action is now. The US nuclear industry is struggling to compete with foreign, state-owned competitors. Any leg-up on competition would be welcomed, including a way to qualify and license reactor systems, fuel and their components in more efficient and cost-effective ways.
3. Advanced reactors will greatly benefit from a new, accelerated fuel qualification process whereas LWRs to a lesser extent, given that their associated Standard Review Plan (SRP) is already well known.

4. Gaps in infrastructure and other resources that are needed to enable optimal application of AFQ to fuel qualification need to be more fully examined.
5. Uncertainties associated with any computational techniques to model or simulate material properties and/or behavior need to be quantified and their implications on validity of m&s results assessed.

4.3 Moving Forward

1. The group agreed on creation of a Technical Working Group (TWG) that would be charged with furthering the development and applicability of the AFQ methodology. The TWG's draft charter should be developed by the next AFQ workshop.
2. All stakeholders are encouraged to continuously communicate with each other on all issues and developments related to AFQ.
3. NRC recommended linking any AFQ-related fuel work to safety analysis activities of the reactor system as a whole (i.e., a holistic approach to safety analysis).
4. The idea of a template to facilitate integration of the AFQ methodology into the NRC regulations was floated and merits exploration.
5. Finding ways to specifically emphasize and facilitate m&s to work hand-in-hand with experiments, in an integrated way, would accelerate establishment of the AFQ methodology. At the agency level, recognize and put resources into developing and assessing it? At the working level, establish and encourage collaborations that couple m&s with experiments?

5 SUMMARY STATEMENT

Accelerated Fuel Qualification (AFQ) is to benefit all stakeholders that are involved in R&D and licensing of new fuels, and relevant technologies, for nuclear energy. The methodology provides a framework to organize efforts among stakeholders with the intent of clarifying interactions and research processes that industries/universities can follow to provide the DOE and NRC with information/data they need for their respective assessments. An agreed-to methodology provides guidance to industry on the path needed to qualify new materials and technologies in an expeditious way that incorporates modeling and simulation with experiments.

6 SPECIFIC NEXT STEPS FOR AFQ

1. Plan for a follow up workshop in the fall 2019 timeframe. The workshop should aim to follow up on items listed in the takeaways above.
2. Establish the AFQ Technical Working Group. This could be discussed and agreed upon in the next workshop meeting.

<u>Specific Terminology:</u>

Integral irradiation tests: Full fuel-cladding irradiations in a test reactor like ATR with similar reactor conditions, or in commercial reactors.

Physics-informed: Use of physics-based modeling to describe physics phenomena instead of empirical fits to data. These models and simulations would need to be tested and found to consistent with experimental data in order to be relied upon for licensing.

Targeted experiments: Those experiments done in conjunction with modeling and simulations to test m&s “predictions”.

APPENDIX A - Accelerated Fuel Qualification (AFQ): Overview

Accelerated Fuel Qualification (AFQ) Workshop
May 31, 2019

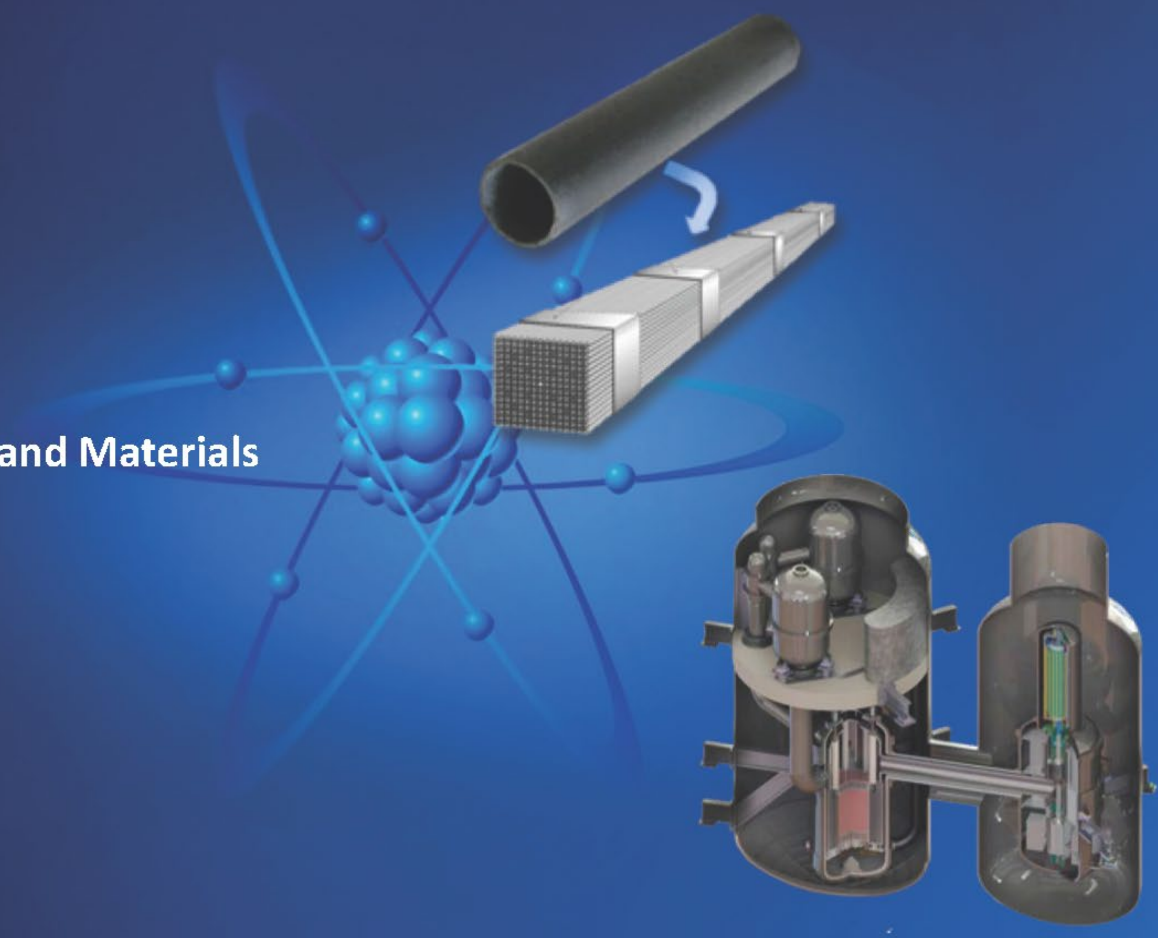
AGENDA

08:30-08:50	**Welcome and introductions**
08:50-09:20	**AFQ Overview: what is AFQ and why is it important?**
09:20-11:00	Example case studies
11:00-11:15	Break
11:15-12:30	Elements of AFQ: DOE Lab capabilities and approaches: Computational & Experimental
12:30-13:30	Lunch
13:30-14:15	NRC perspectives
14:15-15:45	Open discussion
15:45-16:00	Break
16:00-16:45	Next steps
16:45	Adjourn

Accelerated Fuel Qualification (AFQ): Overview

By
Christina A. Back
Ron S. Faibish

Nuclear Technologies and Materials
General Atomics



May 31, 2019

GENERAL ATOMICS

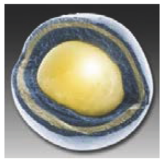
The Proposition

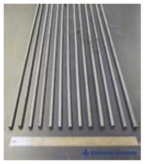
Modeling and experiments must be simultaneously exploited to markedly reduce the years of data that would otherwise be required for deployment of new nuclear fuels.

Why Now: Specific Drivers

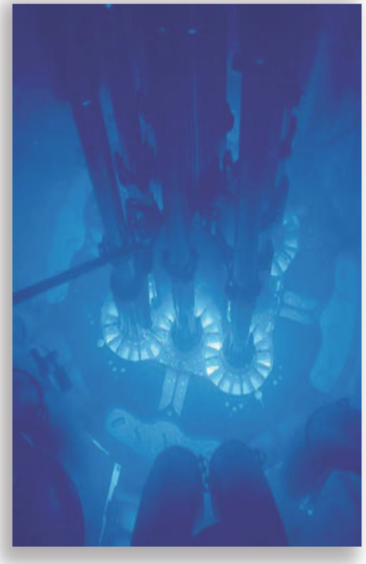
- New non-LWR advanced reactors will require new fuels
  - ✓ e.g., uranium nitride (UN), uranium carbide (UC), liquid molten salt
  - ✓ Higher burnup fuels and long-bure cores

- Currently, it could take more than 20 years and $100s of millions to qualify new fuels
  - ✓ e.g., TRISO, ATF





- Aging, scarce and shutdown test reactors pose a formidable in-pile experimental challenge
  - ✓ Over-subscribed ATR; permanent shutdown of Halden



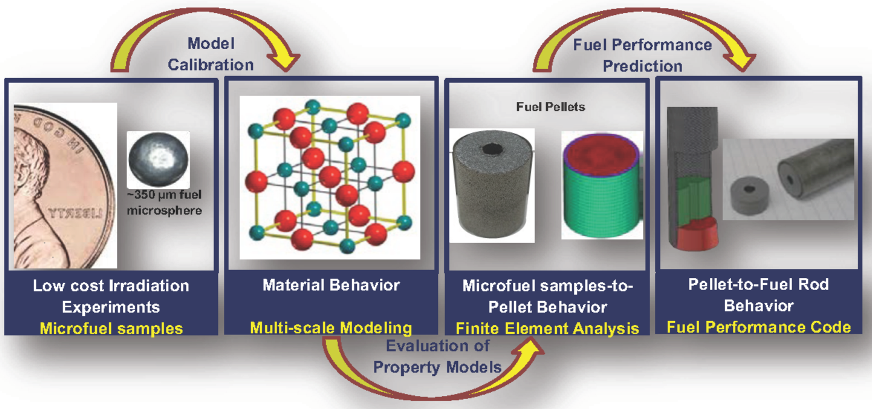
INL's Advanced Test Reactor is over 60 years old – subject to age-related failures

GENERAL ATOMICS

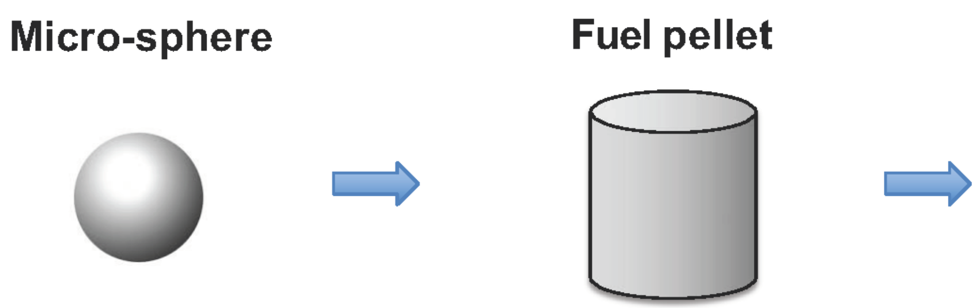
A Key Enabler: Accelerated Fuel Qualification (AFQ)

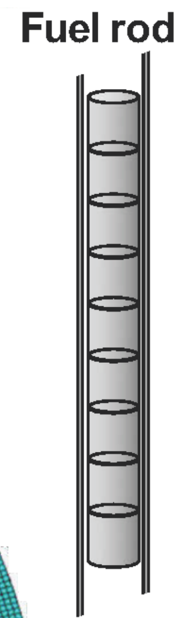
AFQ Defined:

The combination of microstructurally-informed advanced nuclear fuel performance modeling and simulation (M&S) tools with targeted irradiation and other select experimental data that can significantly reduce the cost and number of irradiation experiments and, ultimately, the cost and time associated with new fuel qualification.

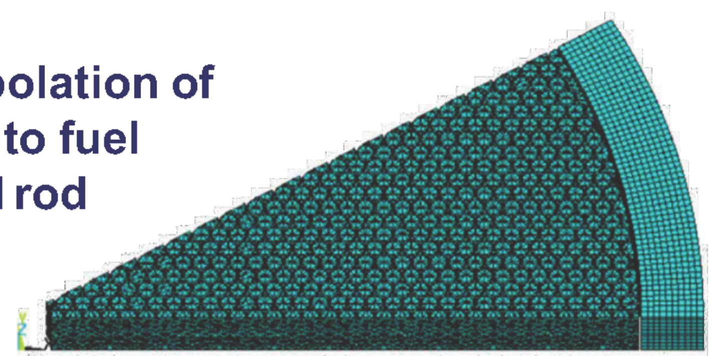


AFQ Takes Advantage of Modeling and Computer Power Advances





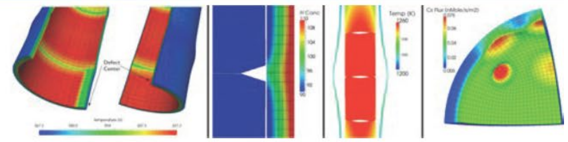
- Computer extrapolation of sphere behavior to fuel pellet and to fuel rod



Approach: Then and Now

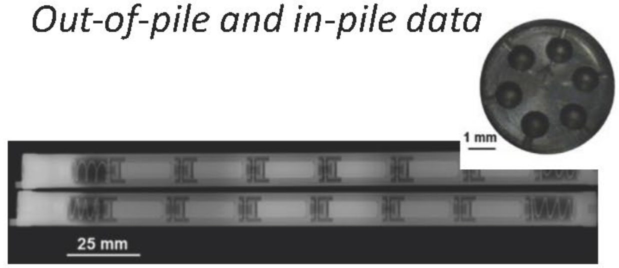
THEN:

- Time-consuming integral tests
- No/minimal use of m&s
- >20 years to qualify/license new fuels



NEAMS

Out-of-pile and in-pile data



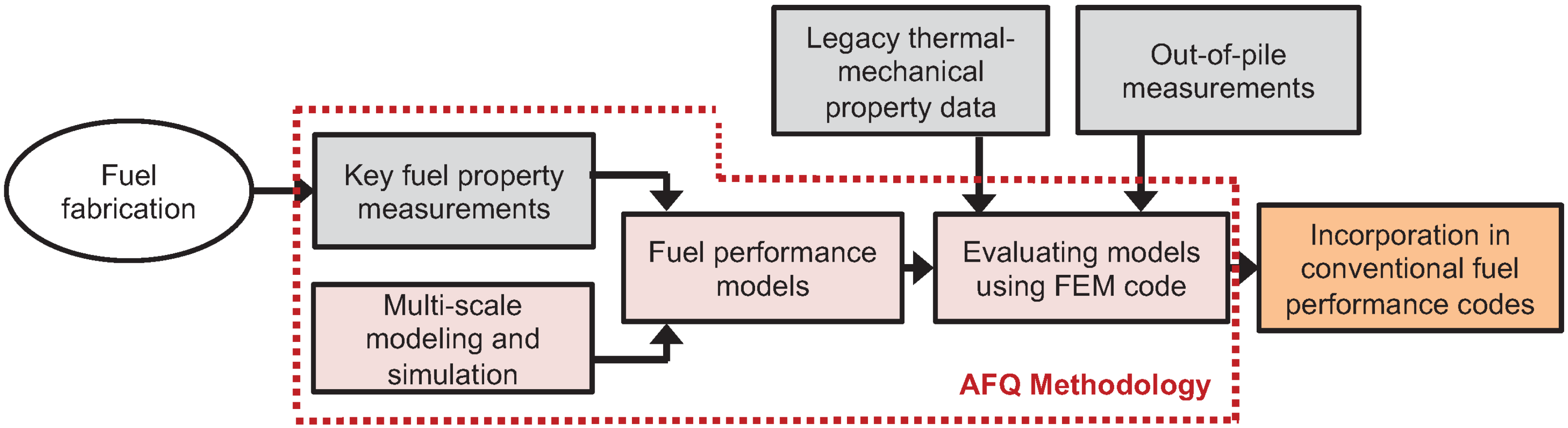
Integral testing at late stage

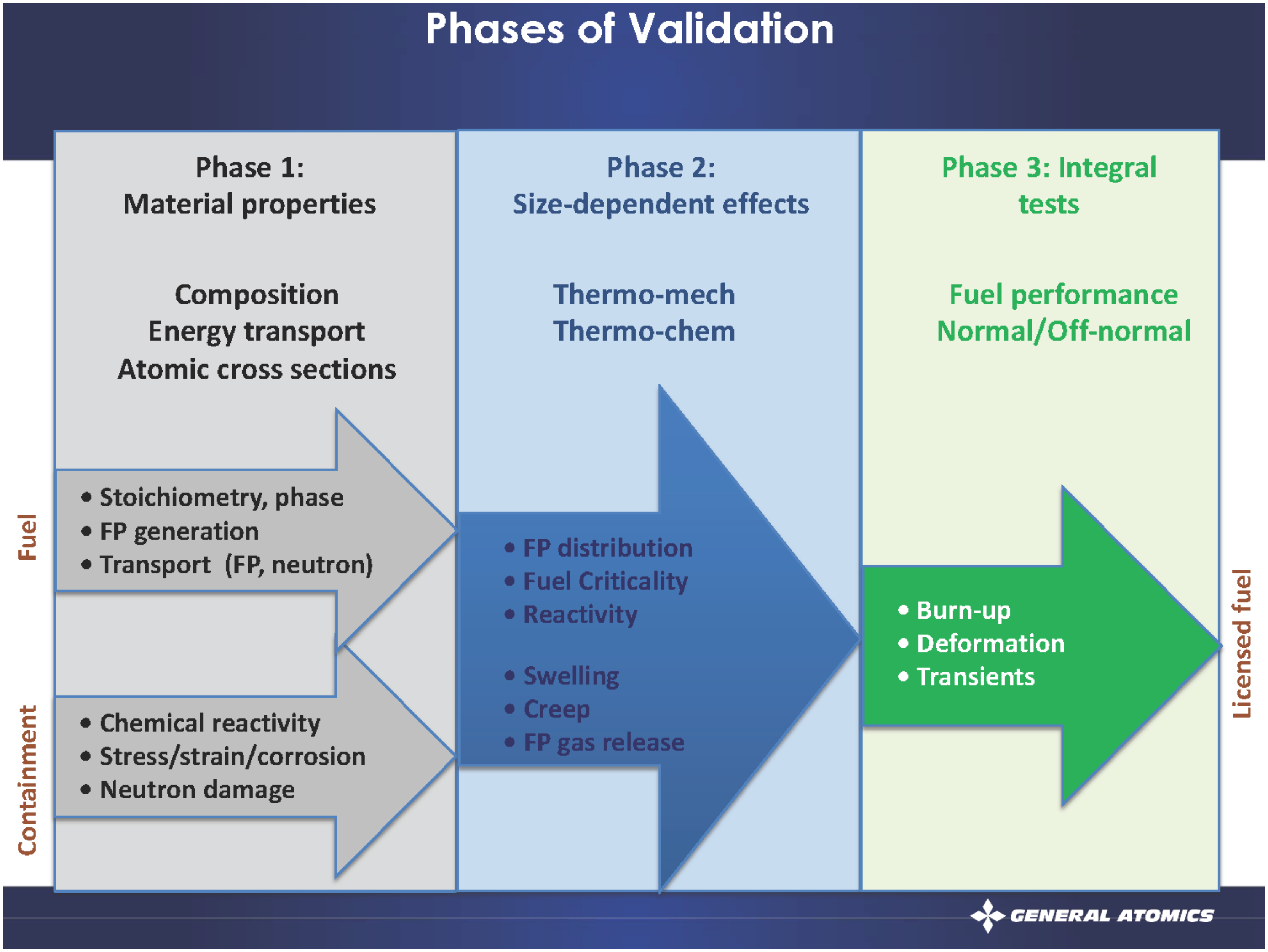
NOW:

- Application of m&s to produce functional fuel designs
- M&S validated by data
- Confirmatory integral testing necessary at late stage
- Goal: <5 years ➔ This is seen as a "Grand Challenge"

Contains contribution by ORNL

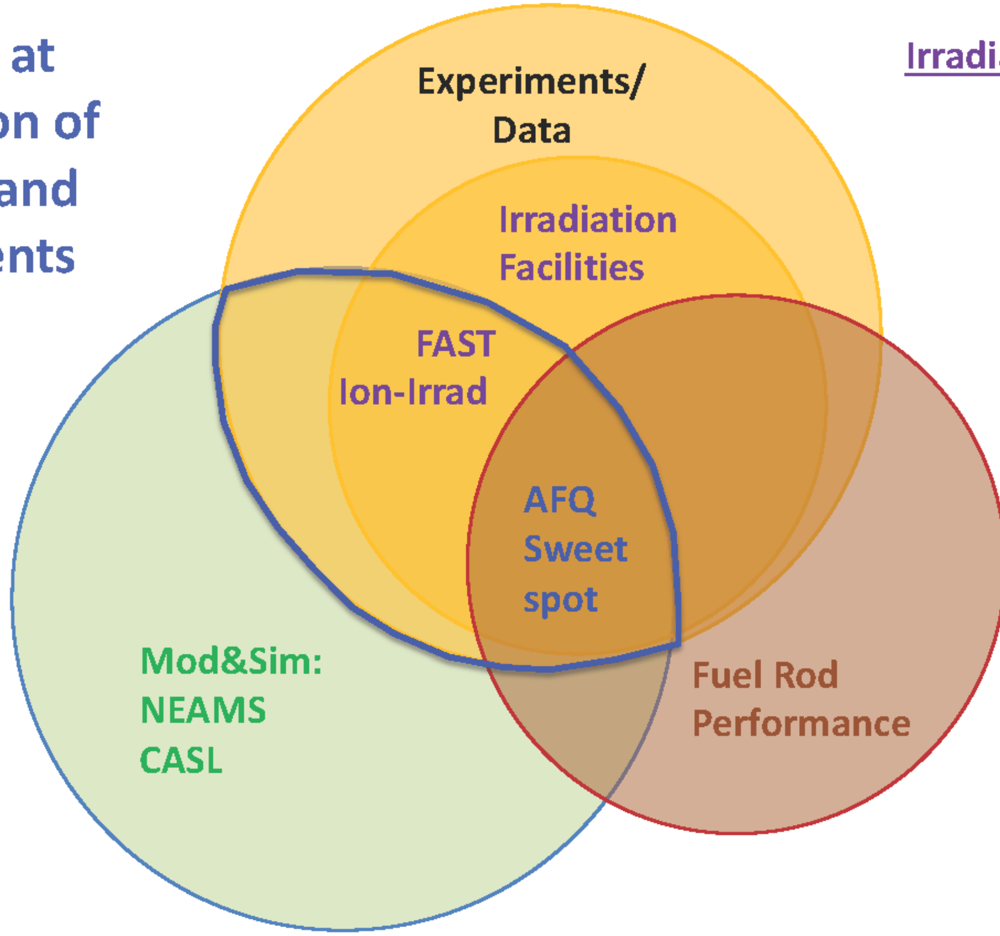
Transition of Advanced M&S Capabilities into Usable Engineering Tools



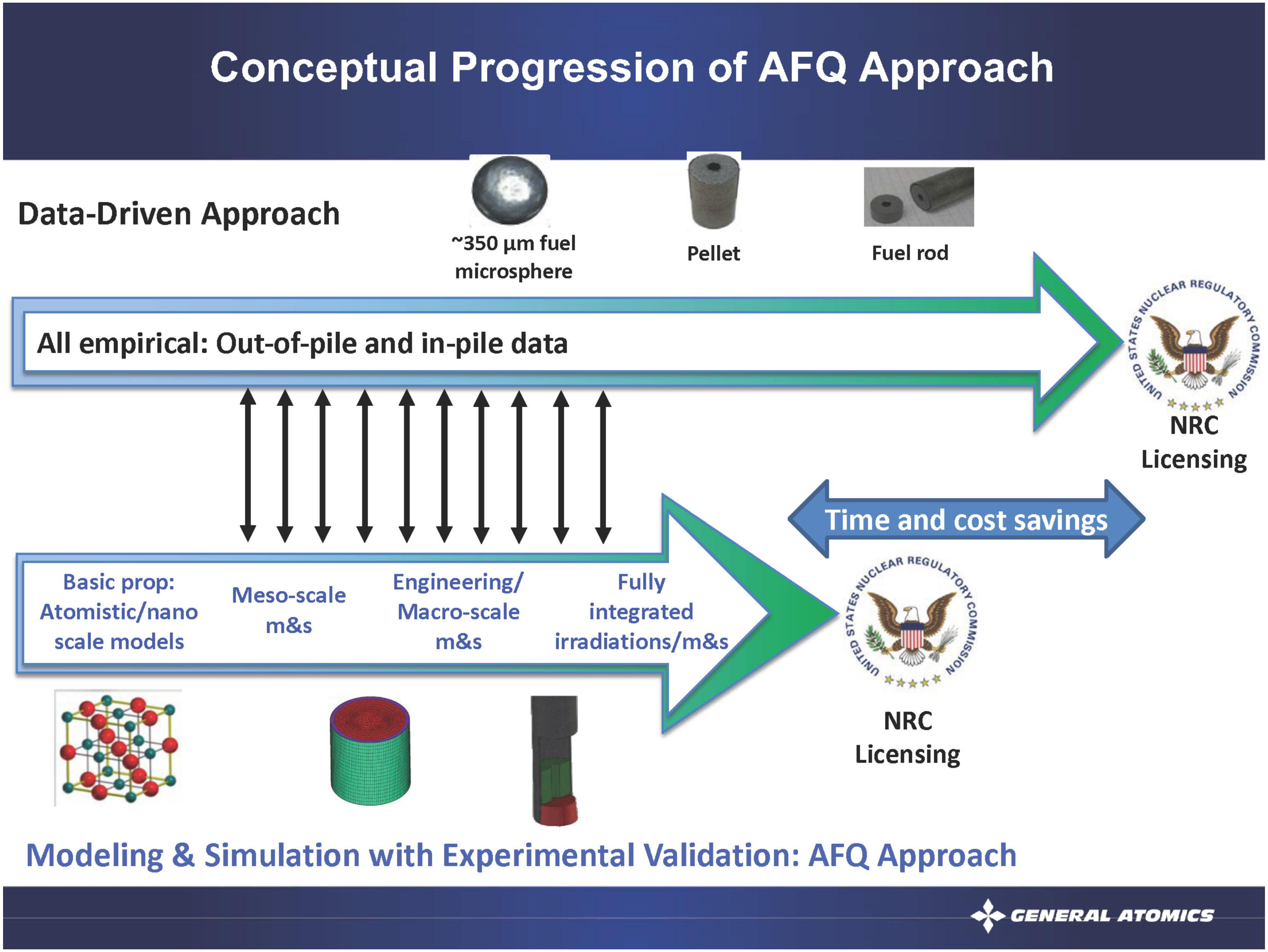

Phases of Validation
Phase 1:
Material properties
Composition
Energy transport
Atomic cross sections
• Stoichiometry, phase
• FP generation
• Transport (FP, neutron)
• Chemical reactivity
• Stress/strain/corrosion
• Neutron damage
Fuel
Containment
Phase 2:
Size-dependent effects
Thermo-mech
Thermo-chem
• FP distribution
• Fuel Criticality
• Reactivity
• Swelling
• Creep
• FP gas release
Phase 3: Integral tests
Fuel performance
Normal/Off-normal
• Burn-up
• Deformation
• Transients
Licensed fuel
GENERAL ATOMICS

Regimes of Relevance in AFQ Methodology

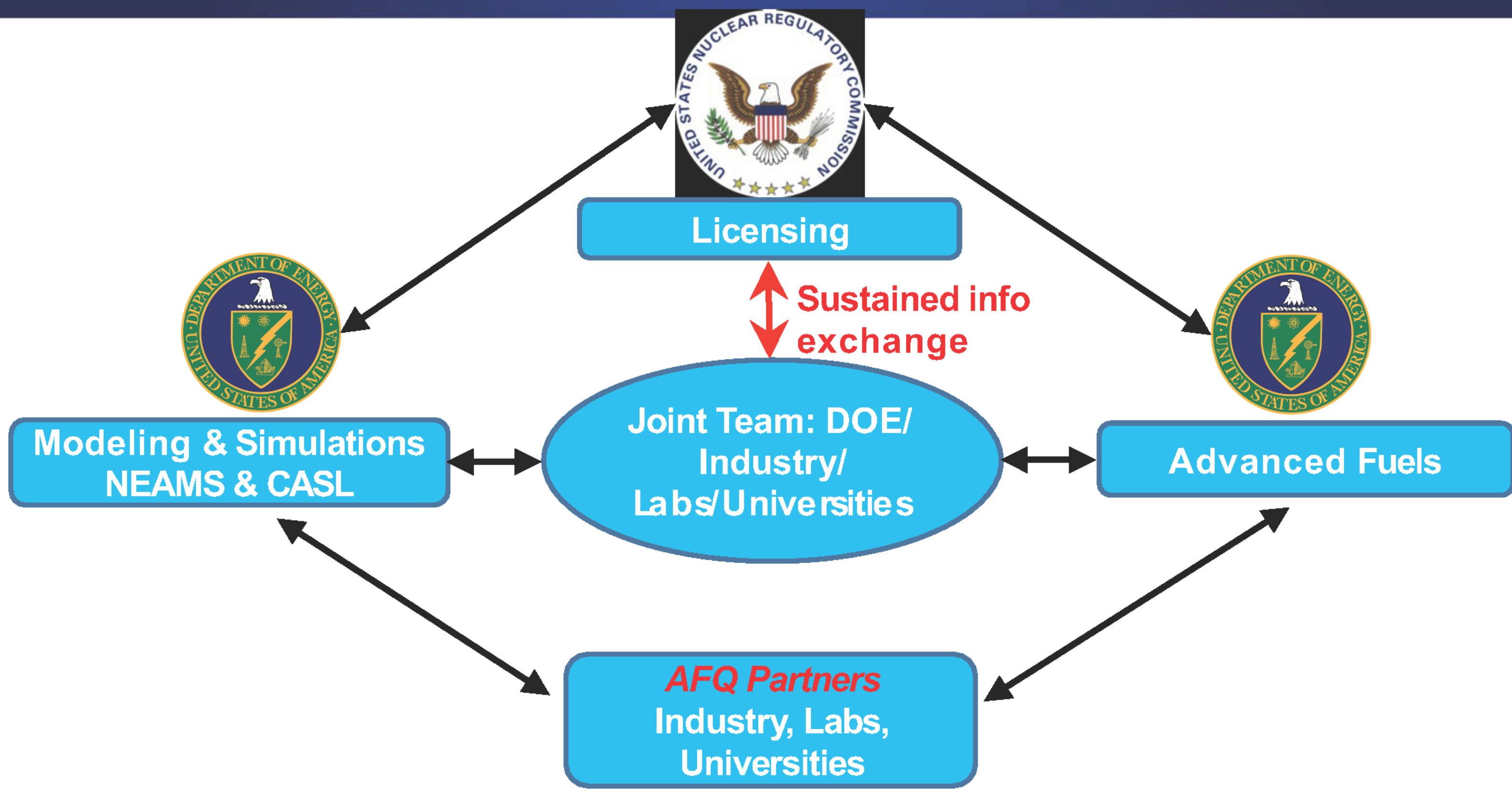
AFQ lies at intersection of ModSim and Experiments



Irradiation Facilities:
ATR
HFIR
MIT-R
TREAT


Conceptual Progression of AFQ Approach
Data-Driven Approach
~350 µm fuel microsphere
Pellet
Fuel rod
All empirical: Out-of-pile and in-pile data
UNITED STATES NUCLEAR REGULATORY COMMISSION
NRC Licensing
Time and cost savings
Basic prop: Atomistic/nano scale models
Meso-scale m&s
Engineering/ Macro-scale m&s
Fully integrated irradiations/m&s
UNITED STATES NUCLEAR REGULATORY COMMISSION
NRC Licensing
Modeling & Simulation with Experimental Validation: AFQ Approach
GENERAL ATOMICS

AFQ Working Framework and Key Stakeholders: Making It All Happen



Building a coalition of partners with DOE's overall coordination

Proposed Next Steps

This workshop is but the first step in a sequence of additional workshops and targeted interactions to assess the path forward.

Next high-level steps:

- **Establish success criteria for AFQ**
  - Development strategy
  - Implementation strategy

- **Determine, and agree upon, a set of high-level consensus milestones to realize success**
  - Deliverables and timeline

Proposed Next Steps (II)

- **DOE's programmatic assistance as an enabler for AFQ development and implementation**
  - What do we recommend as programmatic elements?
  - Resource requirements (e.g., funding, facilities, computing)
- **NRC's stake and interface with all relevant stakeholders**
  - How does this fit with NRC's current efforts?
  - How do we ensure that key success milestones are communicated to the NRC in a timely fashion?
- **How can industry, labs and academia best support DOE and NRC for a constructive engagement on the federal level?**
  - Case Studies– demonstrate the approach
  - NRC engagement with case studies– can this be done informally?

In Conclusion…

When successfully demonstrated and applied, the AFQ approach will open a new horizon for exciting new nuclear fuels to strengthen the competitiveness of the U.S. nuclear industry.

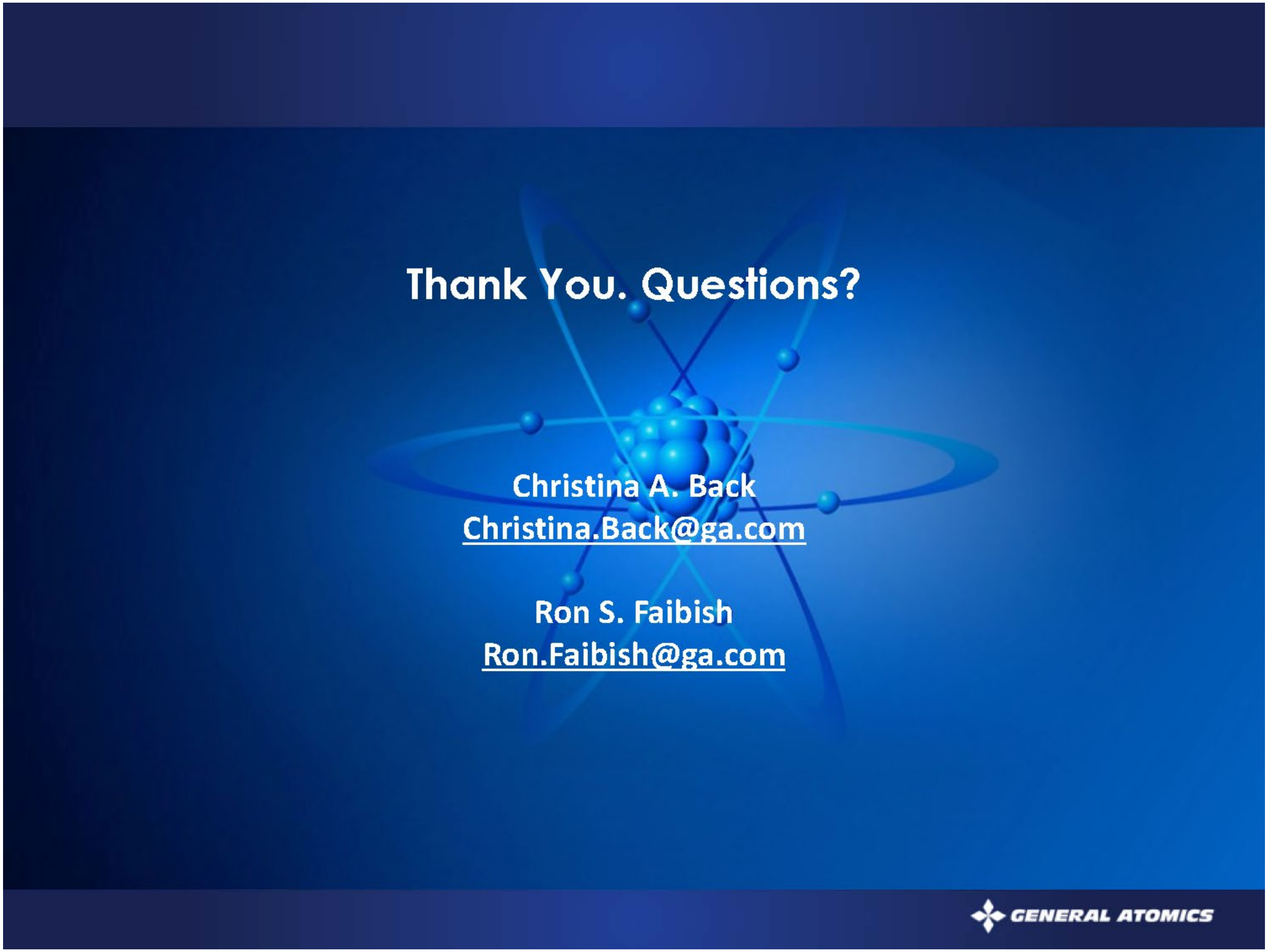
Accelerated Fuel Qualification (AFQ) Workshop
May 31, 2019

AGENDA

08:30-08:50	Welcome and introductions
08:50-09:20	AFQ Overview: what is AFQ and why is it important?
09:20-11:00	**Example case studies**
11:00-11:15	Break
11:15-12:30	Elements of AFQ: DOE Lab capabilities and approaches: Computational & Experimental
12:30-13:30	Lunch
13:30-14:15	NRC perspectives
14:15-15:45	Open discussion
15:45-16:00	Break
16:00-16:45	Next steps
16:45	Adjourn

Learning From Similar Efforts: Case Studies

- **Magnetic Fusion:** Model-based optimization is replacing empirical optimization of fusion fuel (plasma)
- **High Energy Density Plasmas:** Rapidly changing material properties affecting energy transport can be successfully modeled and experimentally validated
- **Mo99 fuel:** When the dominant underlying physics is well-enough described, modeling and simulation can be used in a predictive way (extrapolation)
- **SiC composite:** When behavior of constituent properties are understood over a range, modeling and simulation can be used to engineer properties of materials (interpolation)
- **UC Fuel:** Validating models of fission gas release and swelling are critical to determining future “targeted” experiments


Thank You. Questions?
Christina A. Back
Christina.Back@ga.com
Ron S. Faibish
Ron.Faibish@ga.com
GENERAL ATOMICS

APPENDIX B - Appendix B: AFQ Case Studies

AFQ Case Studies

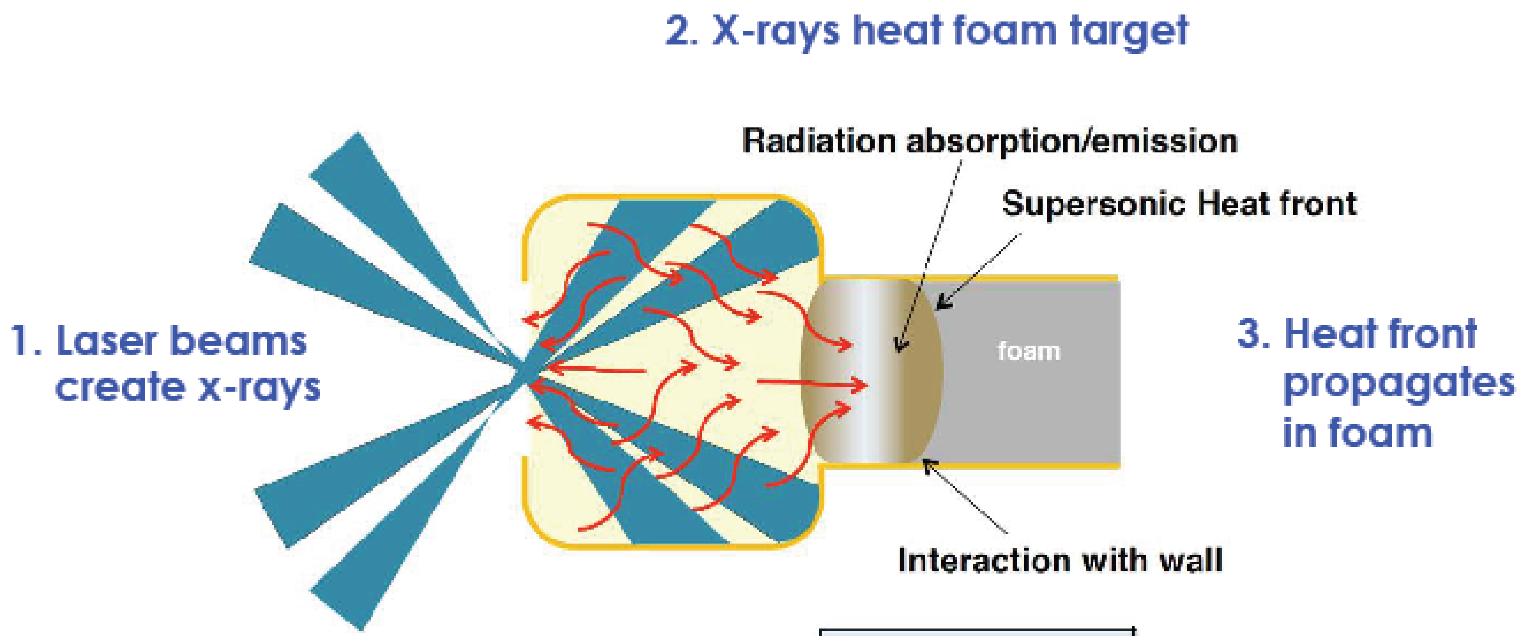
By
Christina Back
General Atomics
Nuclear Technologies
and Materials

To
AFQ Workshop

May 31, 2019

GENERAL ATOMICS

Experiments Must Be Sufficiently Constrained To Benchmark Models



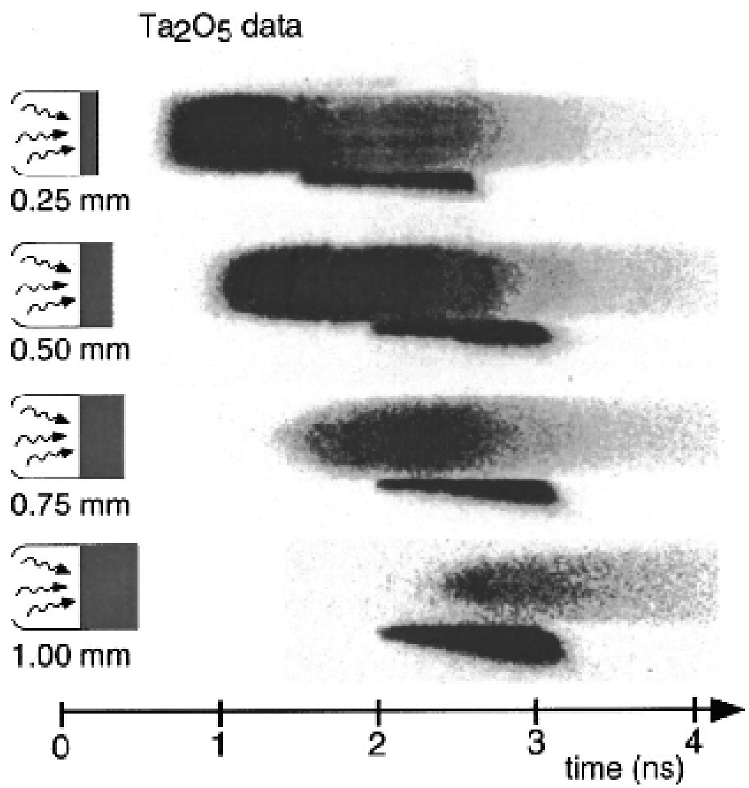
$$x \approx \sqrt{\frac{\sigma T^4 t}{\kappa \rho^2 \varepsilon}}$$

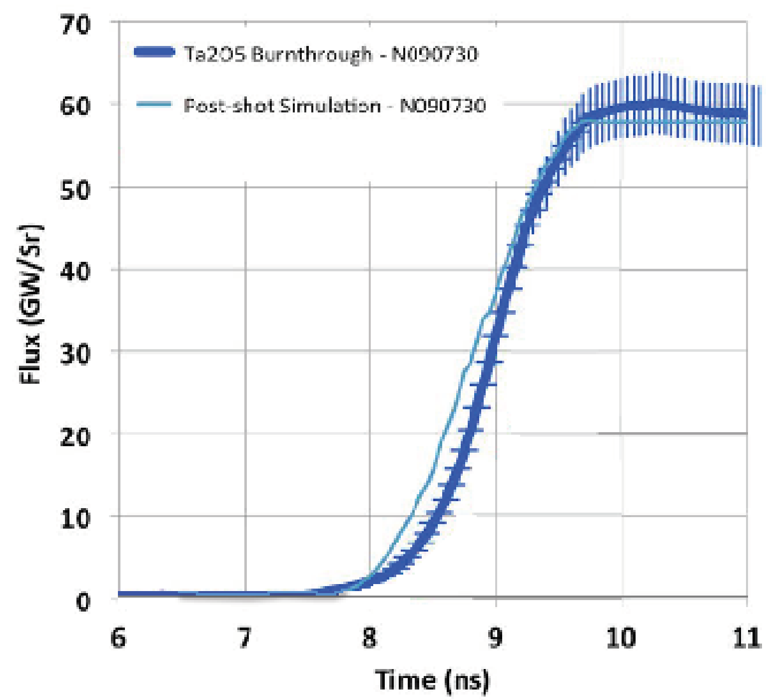
propagation

NIF

GENERAL ATOMICS

Breakout Time of the Heat Wave Is a Sensitive Observable





Back, et al, PRL 84, (2000); Phys. Plasmas 21 (2000)

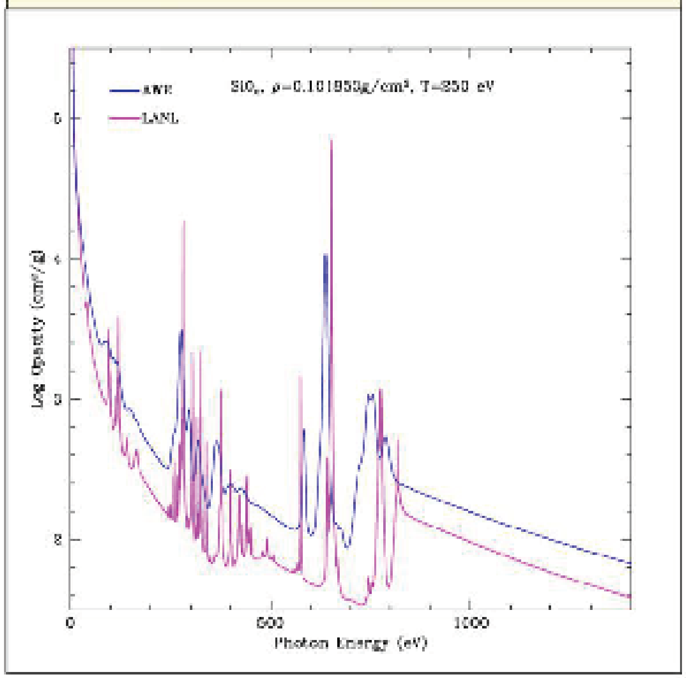
Moore, et al, Phys. Plasmas 21, (2014)

GENERAL ATOMICS

Opacity Is One of Many Variables That Affect Radiation Transport

Opacity models for SiO2 differ by 65% over the range of 300-600 eV

SiO_2 Opacity (ρ=0.1g/cc, T=250eV)



Opacity calculation from C. Fryer (LANL)

- **Difference between opacity models → 300ps difference in radiation wave arrival**
- **Code-to-code comparisons between AWE and LANL, show ≈1ns uncertainty in predicting the arrival time.**

NIF

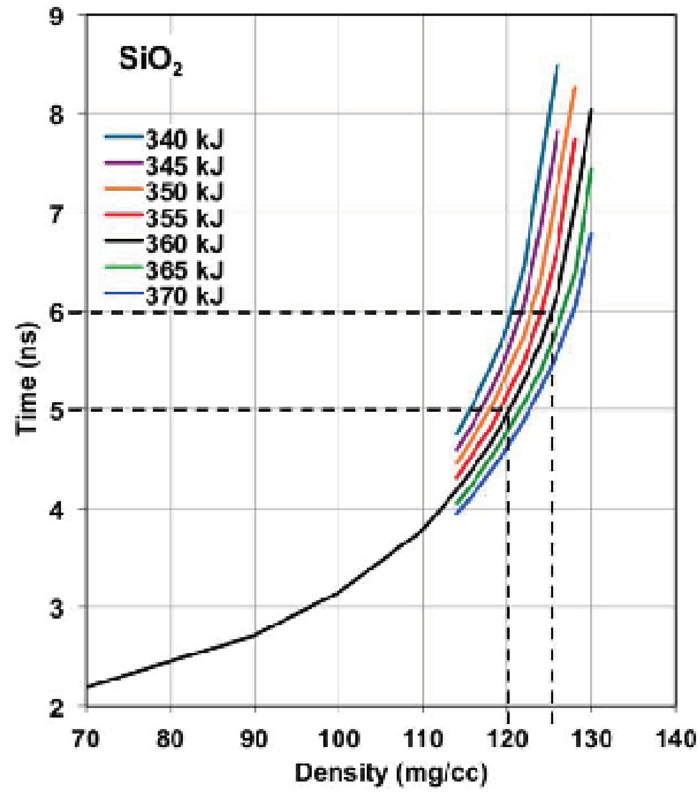
GENERAL ATOMICS

Simulations "Define" Optimal Parameters and Error Bars For Experiments

- The foam-tube length was optimised to create the highest sensitivity to opacity and EOS while remaining super-sonic.

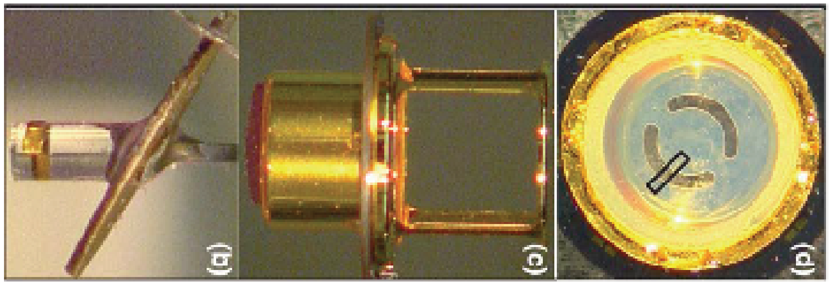
- Simulations show the non-linear behaviour characteristic of the radiation wave approaching the transition from super- to sub-sonic at the end of the tube.

A 5mg/cc (4%) change in foam density results in a 1ns change in arrival time; this is equivalent to a 16% difference in opacity

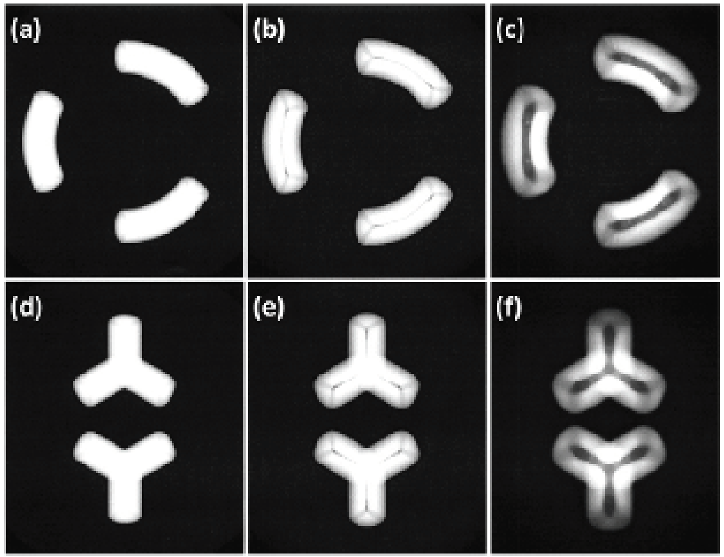


Moore, et al, 20th ICF Target Fabrication Meeting, (2012)

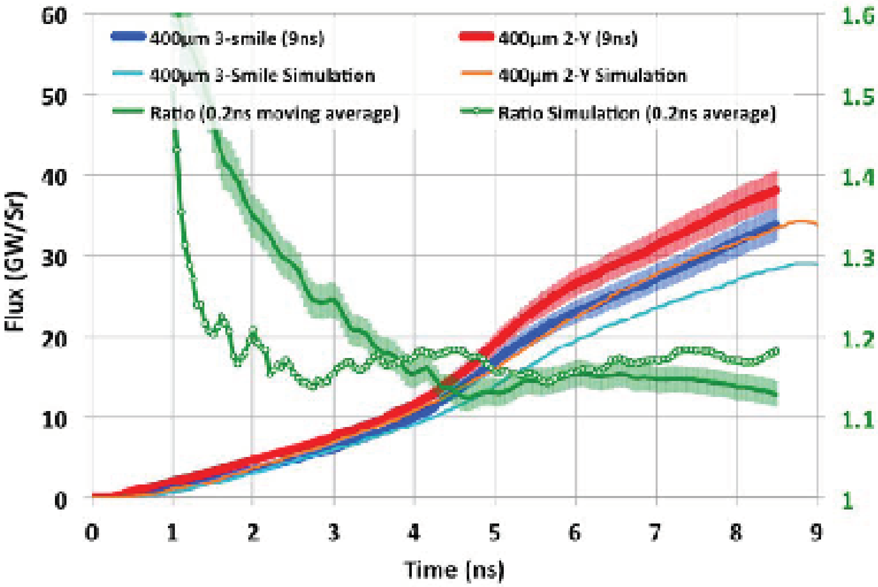
Energy Transport Experiments and Simulations Are In Excellent Agreement Before Plasma Filling



- **Free-streaming and diffusive transport**
  - Measured by calorimetry
  - Modeled by Monte Carlo transport modeling



Simulated radiographs



7 Cooper, et al, Phys. Plasmas 20, (2013) GENERAL ATOMICS

Case Study: Radiation Transport

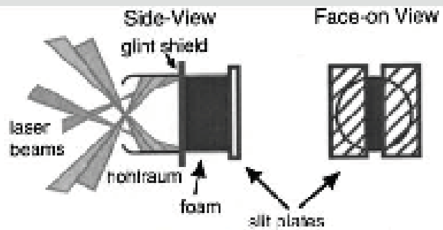
- **High energy density plasmas:**

  Rapidly changing material properties affecting energy transport can be successfully modeled and experimentally validated
  - US nuclear weapons are certified

Radiation Transport Platform Allows For Investigation Of Multiple Phenomena

Hohlraum driven foams and aerogels enable the study of a wide range of radiation transport physics

Radiation transport in materials

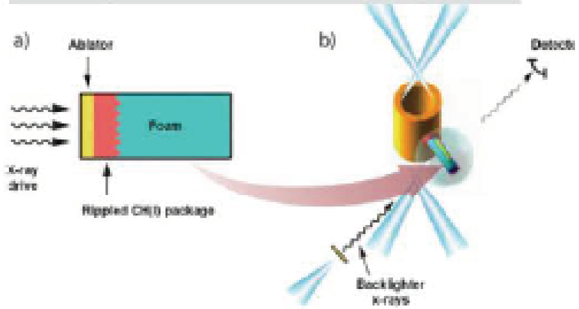


C. A. Back *et al.*, Phys. Plasmas 7, 2126 (2000)

Radiation transport in non-uniform materials

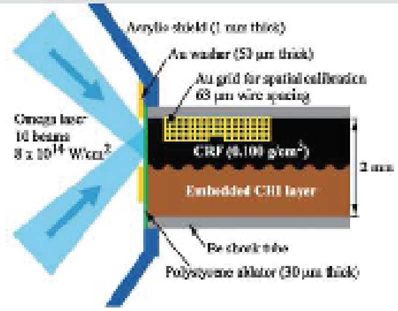
P. A. Keiter *et al.*, Phys. Plasmas 15, 056901 (2008)

Super nova core collapse



C.C. Kuranz, *et al.* Astrophys. Space Sci. 336, 207 (2011)

Kelvin-Helmholtz Instability



E. Hardin, et al. PRL 103, 045005 (2009)

GENERAL ATOMICS

APPENDIX C - SiC Composite

SiC Composite: An Engineered Material Example Using a Constituent Model

SiGA

ANSYS model is used to predict mechanical strength based on braid architecture

- Model complex multi-layer braid architectures
- Matrix densification must be considered
- Use constituent properties/models to get macro behavior

Define Architecture **Grow in Fiber** **"Deposit" Matrix**

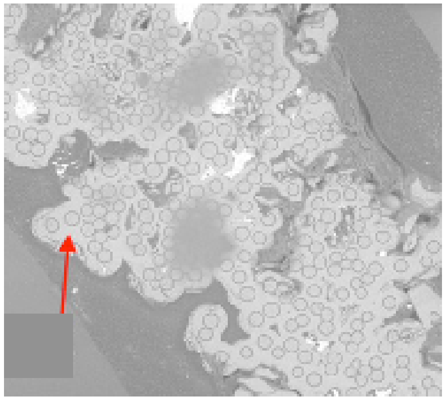
GENERAL ATOMICS

Constituent Properties That Are Important To Predict Macro Behavior

- **Fibers treated as infiltrated tow bundle**
  - Data taken from experimental single tow testing
  - However…this could be treated as fiber filament/PyC Interphase/SiC infiltration sub-model
- **Matrix as monolithic SiC with micro porosity correction**

Input Data for Fiber Tow (In Axis)

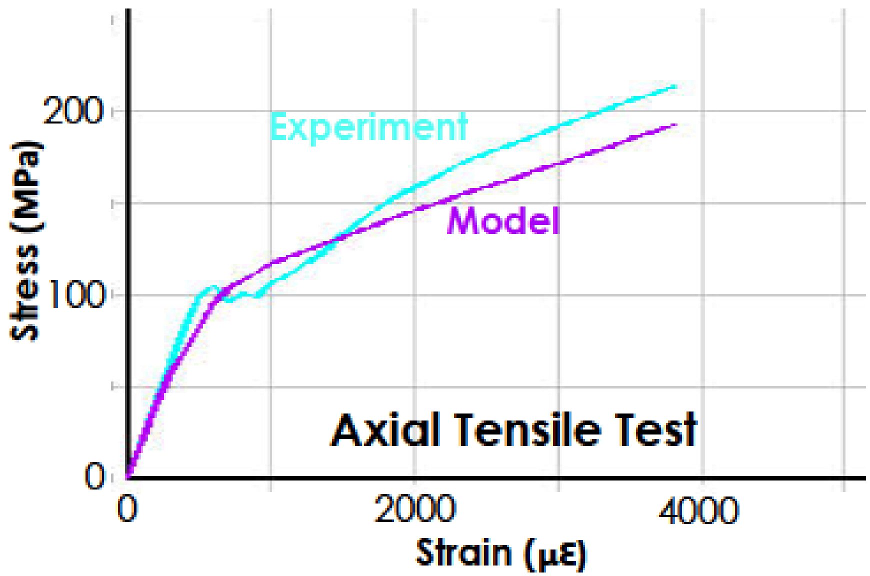
Property	Value
Dimensions	1.25 x 0.15 mm
Elastic Modulus	301 GPa
Tangent Modulus	61 GPa
PLS Strain	0.16 %
Failure Strain	0.80 %



Almansour, et al, J. Europ Ceramic Soc, 35, 2015

Model Validated Via Experimental Test Data

Model validated by comparing PLS stress/strain and UTS stress/strains for three different braids to existing experimental data



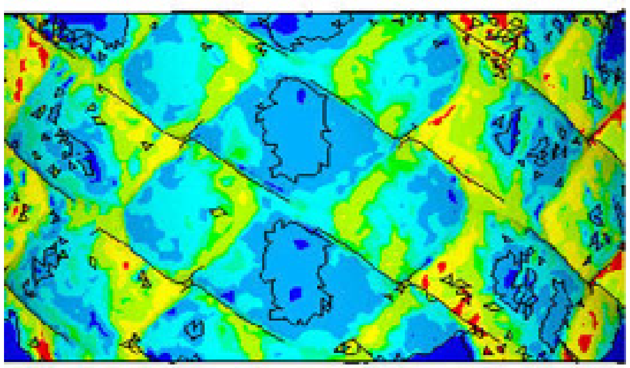
Deviation Between Model and Experimental Data				
Braid	Axial PLS	Axial UTS	Hoop PLS	Hoop UTS
A	6%	9%	21%	14%
B	24%	22%	12%	16%
C	2%	8%	24%	8%

GENERAL ATOMICS

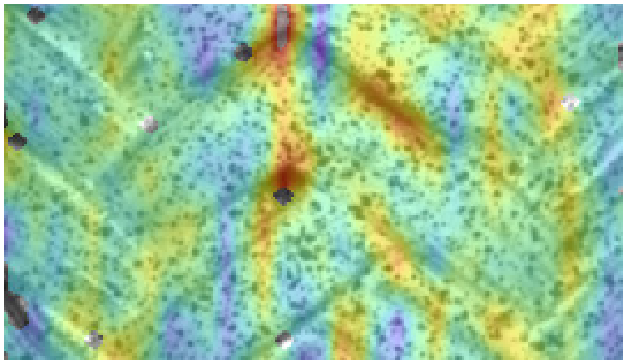
Predicted Behavior Confirmed, Model Extended

- **Model used to predict behavior for a unique, previously untested braid architecture**
  - Composite tube was then fabricated and tested
  - Agreement within 20% of model

- **Push the limits of the model -> Prediction of localized strain behavior**



Model



Experimental (Digital Image Correlation)

Case Study: SiC Composite

- SiC composite:

  When behavior of constituent properties are understood over a range, modeling and simulation can be used to engineer properties of materials (interpolation)

  – Define range for targeted irradiation testing

APPENDIX D - MO-99 EXAMPLE

Mo99: UO_2 Modeling Extrapolated To Higher Enrichment Was Successful At Predicting Fuel Behavior

Challenge: Design/fabricate a UO_2-zircally fuel system with
5 times the power density and
3 times the heat flux of a PWR fuel rod

Key parameters of concern:

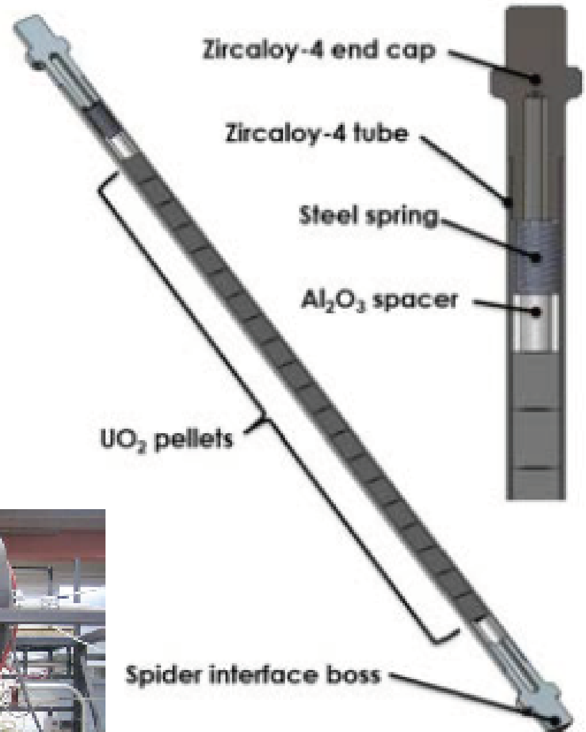
- Critical heat flux margin
- Fuel centerline temperature
- Fission gas release
- Cladding strain

Design approach: Modified FRAPCON for geometry, enrichment, temperature near melting

Program schedule was such that we had to get it right the first time

Mo99 System Design for Selectively Extracting Isotopes From Uranium Fission

- **Mo99 system design**
  - High enrichment
  - Higher heat flux
  - Smaller diameter
- **Modeling adaptations**
  - Corrected radial power profile
  - Added Bernath CHF
  - Adapted thermal boundary conditions



Mo99 Fuel Analytical Predictions and Data

Critical heat flux (U. of Wisconsin)

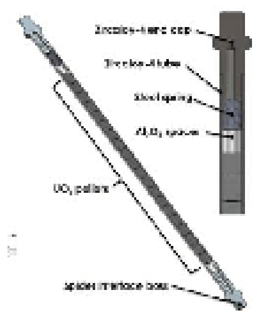
Inlet T, °C	Mass flux, kg/s-m2	Meas. CHF, MW/m^2	Pred. CHF, MW/m
32.5	5000	9.24	9.6
33.8	4250	8.60	8.3

Fuel centerline temp. (CNL reactor)

Metallographic exam - ~2500°C Predicted 2459°C

Fission gas release (CNL reactor)

FGR (%)	2-Week Irradiation		3-Week Irradiation	
	FRAPCON	Test	FRAPCON	Test
Position 3	11.6	13.6 ± 2.2	29.9	31.1 ± 5.2
Position 4	8.2	11.5 ± 1.9	26.9	25.2 ± 4.3



Cladding strain (CNL reactor)

Permanent Hoop Strain (%)	2-Wk Irradiation	3-Wk Irradiation
Position 3	0.03	0.29
Position 4	-0.00	0.06

Takeaway: modeling was remarkably accurate – save significant time

Case Study: Mo99

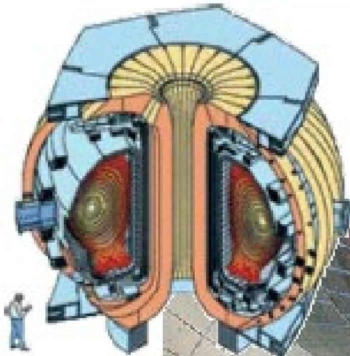
- **Mo99 fuel:**

  When the dominant underlying physics is well-enough described, modeling and simulation can be used in a predictive way (extrapolation)

  – i.e. less testing between 5 and 19 % enrichment

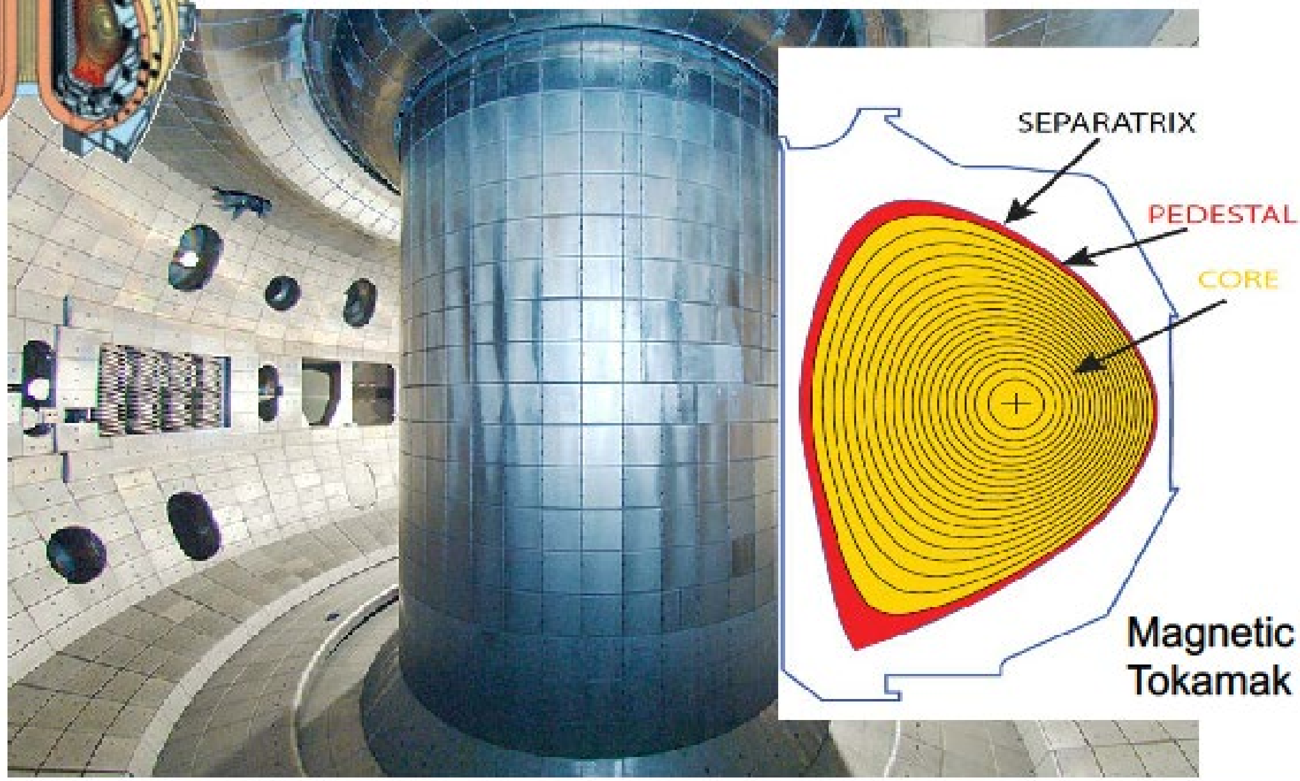
APPENDIX E - Appendix E: FUSION EXAMPLE

Magnetic Fusion Energy: Pedestal Optimization



Magnetic fusion confinement critically depends on the pedestal

DIII-D NATIONAL FUSION FACILITY SAN DIEGO

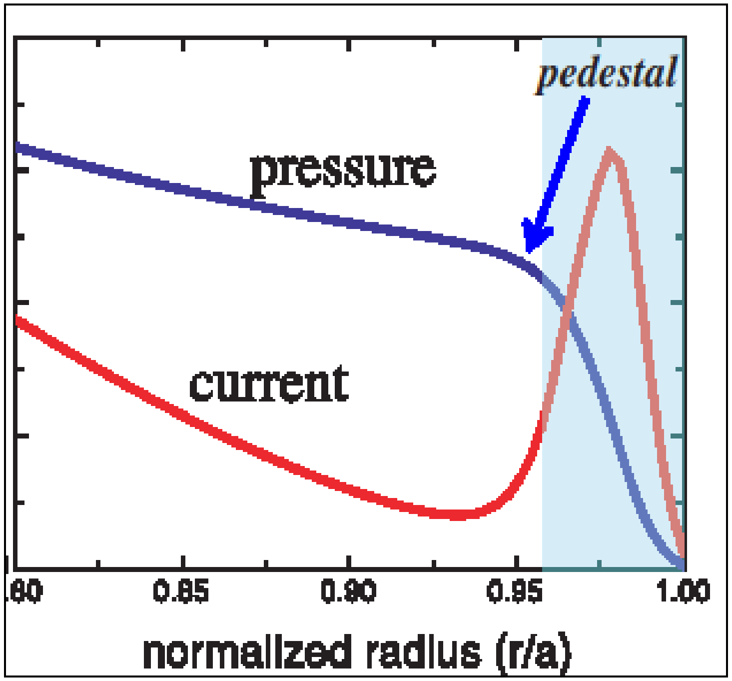


Magnetic Fusion Tokamak Plasma

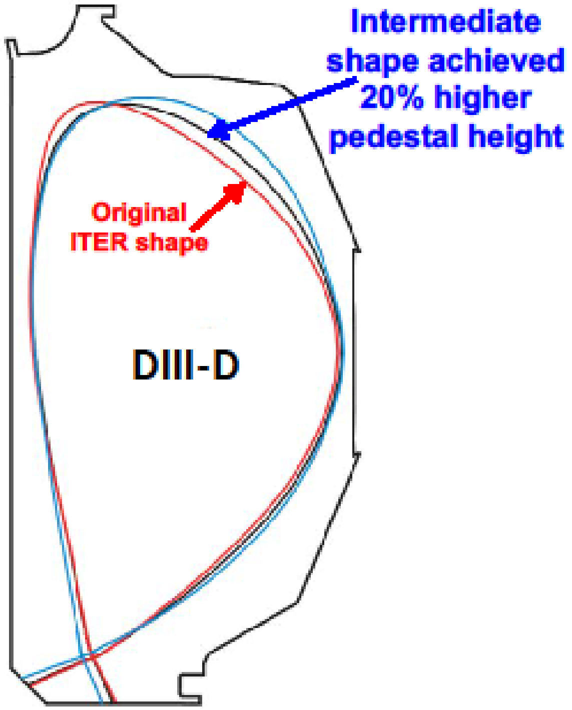
GENERAL ATOMICS

An Empirical Approach Was Used To Determine the Plasma Shape for ITER

- In H-mode regime, a "pedestal" forms near the edge of the confined region



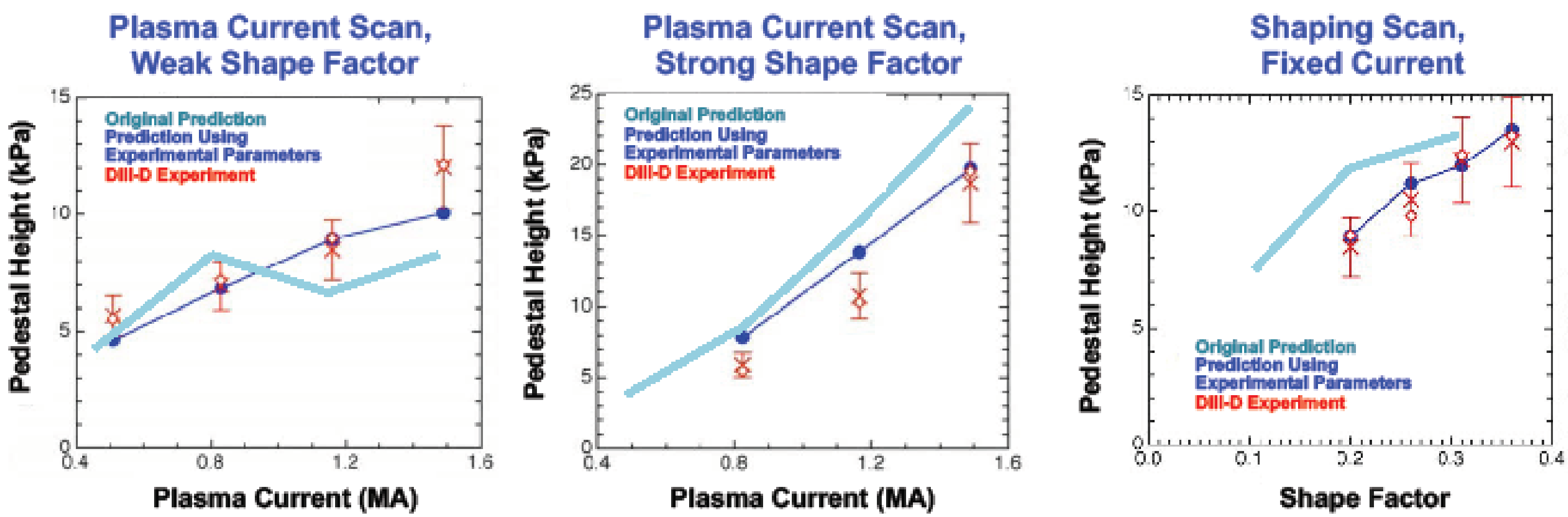
- Empirical studies showed distinct sensitivity to plasma "shape"



GENERAL ATOMICS

Models Identified Key Variables and Experiments Were Performed Over the Critical Parameter Range

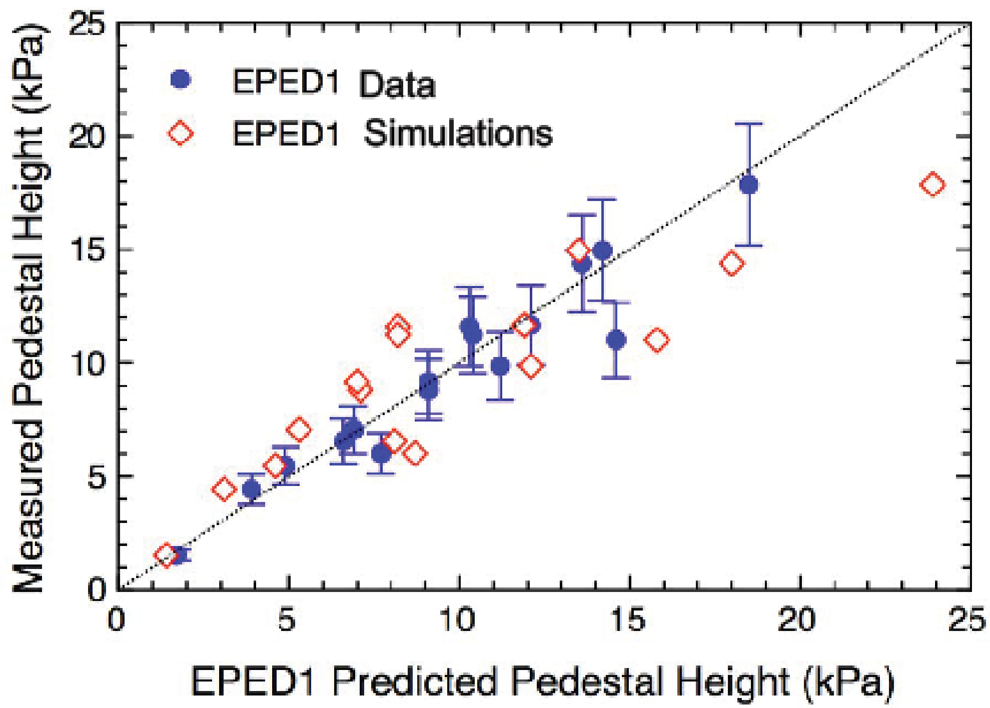
- **Data did not initially match original predictions because input conditions were not exactly matched**



- **Post-analysis using actual experimental conditions improved the match**
- **Iteration with experiments led to refined models**

GENERAL ATOMICS

Model Predicts Pedestal Height Correctly Over an Order of Magnitude Range in Performance Quality



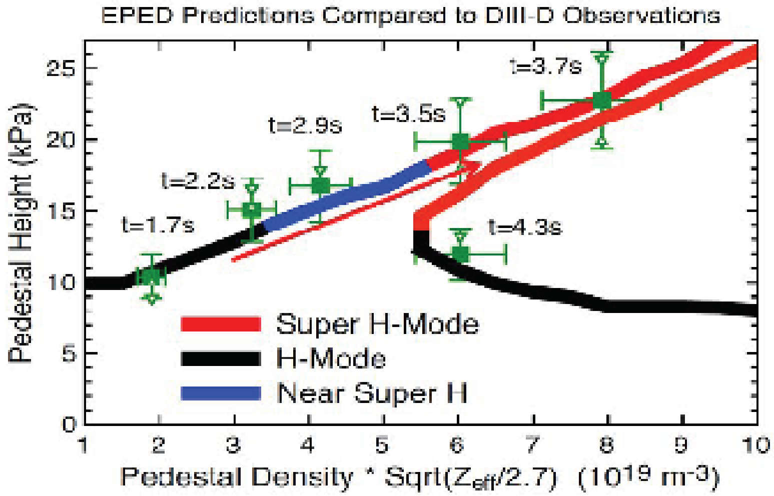
Model accurately reproduces key trends
→ Now use model to optimize performance!!!

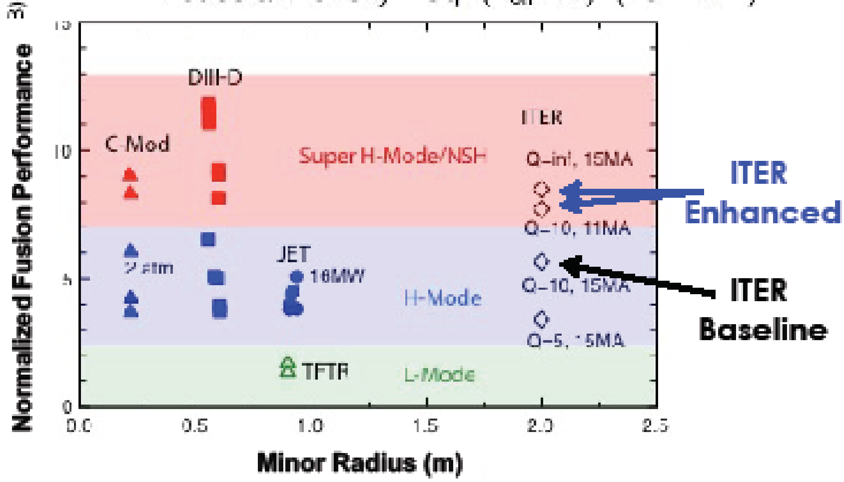
GENERAL ATOMICS

The Super H-Mode Regime Was Predicted By Modeling and Simulation, and Confirmed By Experiment

- **Through improvements in model (EPED1→ EPED1.6) experiments, confidence in model grew**
- **Super H-mode regime**
  - Improved edge-peeling ballooning stability
  - Requires strong shape factor with high plasma density
- **Experiments in DIII-D and C-Mod have confirmed the Super H-mode**
  - ITER may be able to exceed its design objectives

Model-based exploration led to pedestal optimization





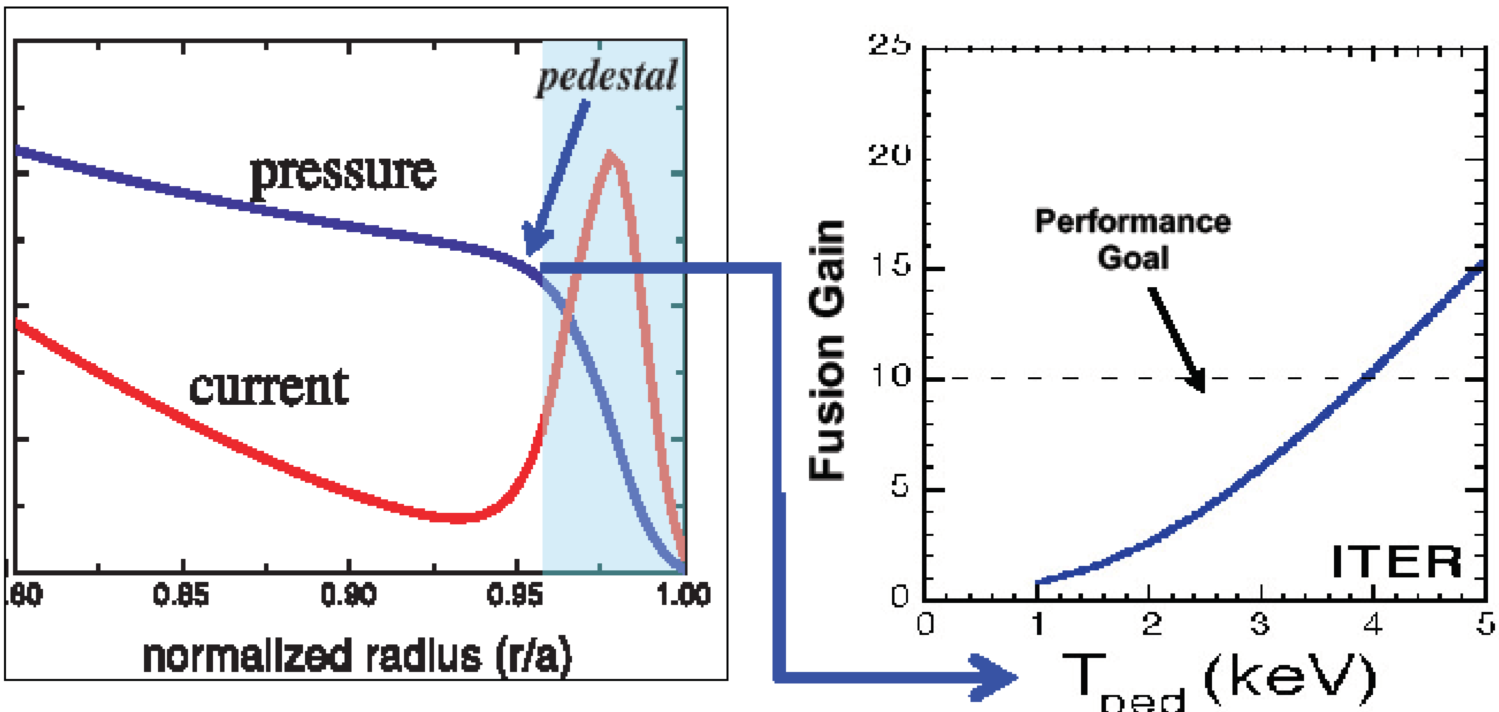
Case Study: Magnetic Fusion

- Magnetic fusion energy:

  Model-based optimization is replacing empirical optimization of fusion fuel (plasma)
  - Higher fusion gain is achieved with fewer experiments

Models Started to Show Critical Impact of the Pedestal Height on Tokamak Performance

- In H-mode regime, a "pedestal" forms near the edge of the confined region
- Fusion performance is critically dependent on the pedestal

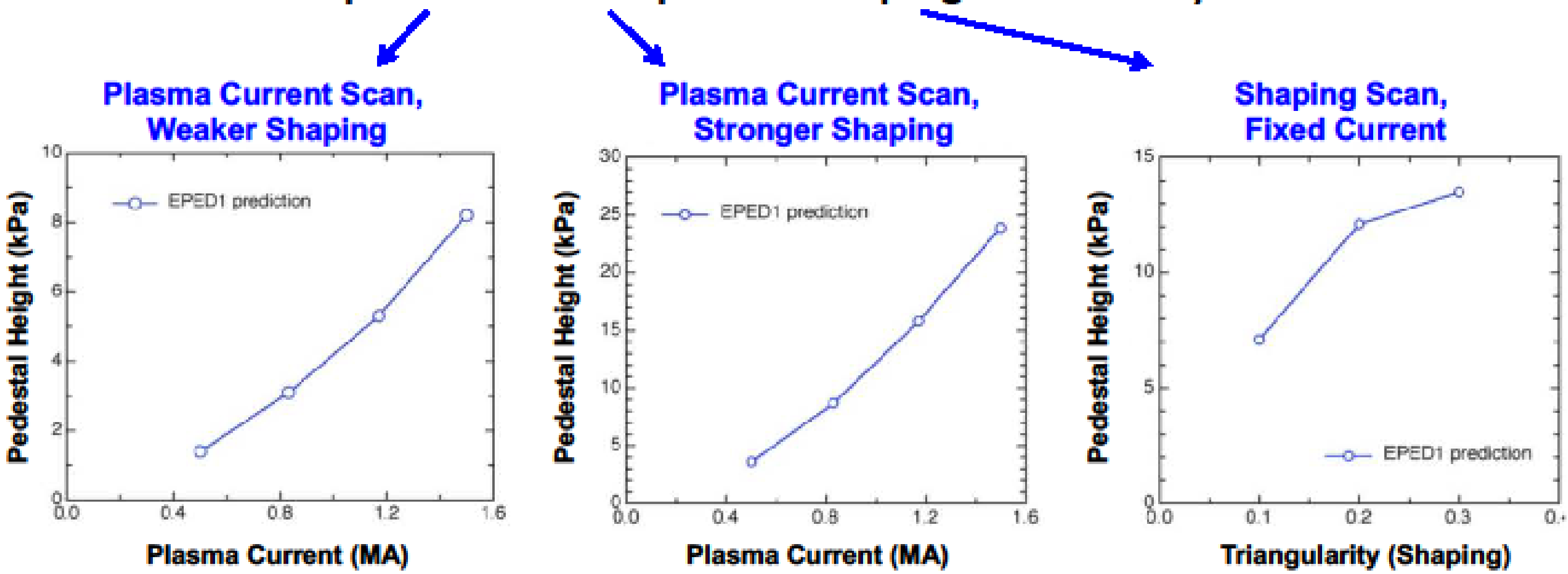


Modeling and simulation provide insight into how to control the plasma

GENERAL ATOMICS

Initial Modeling Identified Key Variables Controlling Pedestal Performance

- EPED1 (Pedestal Stability Code, 2008) identified plasma current, plasma shaping, and density



Experiments were undertaken to confirm the key dependencies

GENERAL ATOMICS

APPENDIX F - Appendix F: UC Irradiation Project

UC Irradiation Project

Validating models of fission gas release and swelling are critical to determining future “targeted” experiments

GENERAL ATOMICS

Why UC?

- UC/SiC has been chosen as the baseline fuel for a GA-developed high-temperature helium-cooled fast reactor known as the Energy Multiplier Module (EM^2)

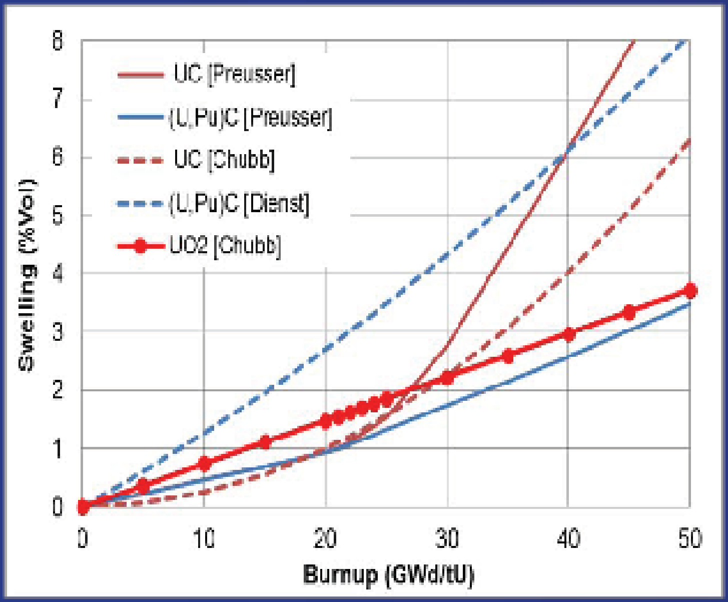
- UC is an important advanced reactor fuel because of its attractive thermal-physical properties

- Highly compatible with silicon carbide (SiC) composite (SiC-SiC) SiGA™ cladding

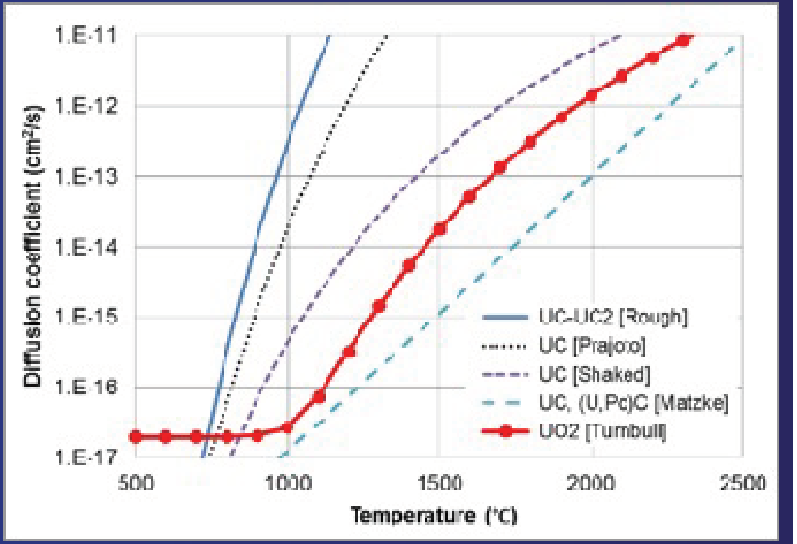
- GA has developed and demonstrated a commercially viable process for manufacturing high-quality UC fuel

- **The proposed effort demonstrating the AFQ methodology is the first step towards qualifying UC fuel**

Specific Motivation for AFQ: Inconsistent UC Data



UC swelling compared to UO_2



UC diffusion coefficients compared to UO_2

GENERAL ATOMICS

GA's Two-Year DOE Contract to Begin Demonstrating AFQ

Project is only the first step

Develop and demonstrate AFQ for irradiation-induced swelling and fission gas release in EM^2 UC fuel rod

Future steps

Develop and confirm models for other fuel performance properties, such as pellet clad mechanical and chemical interactions

Project Participants

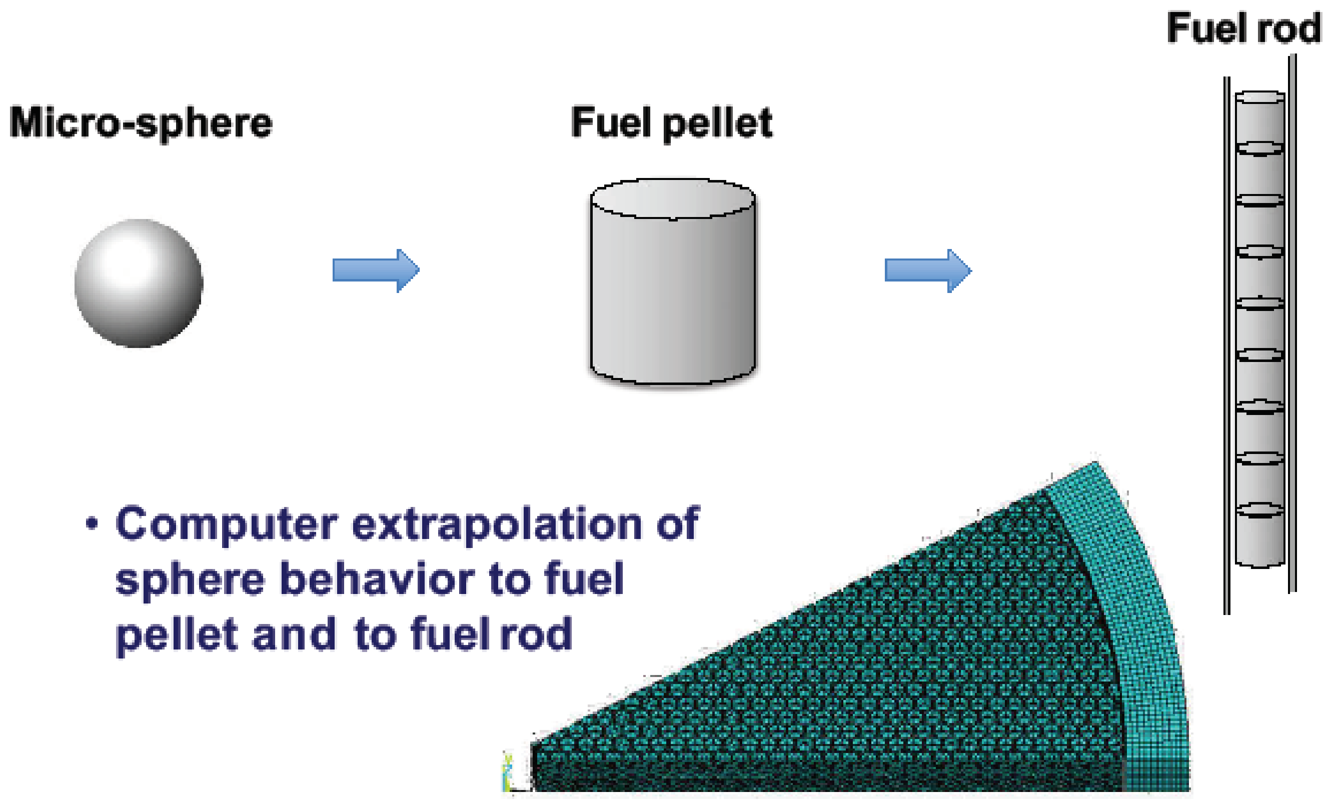
Oak Ridge National Lab – irradiate microsphere in HFIR and perform PIE

U. of Tennessee (Knoxville) – multi-scale modeling of sphere

GA – make fuel samples and perform continuum scale-up analyses

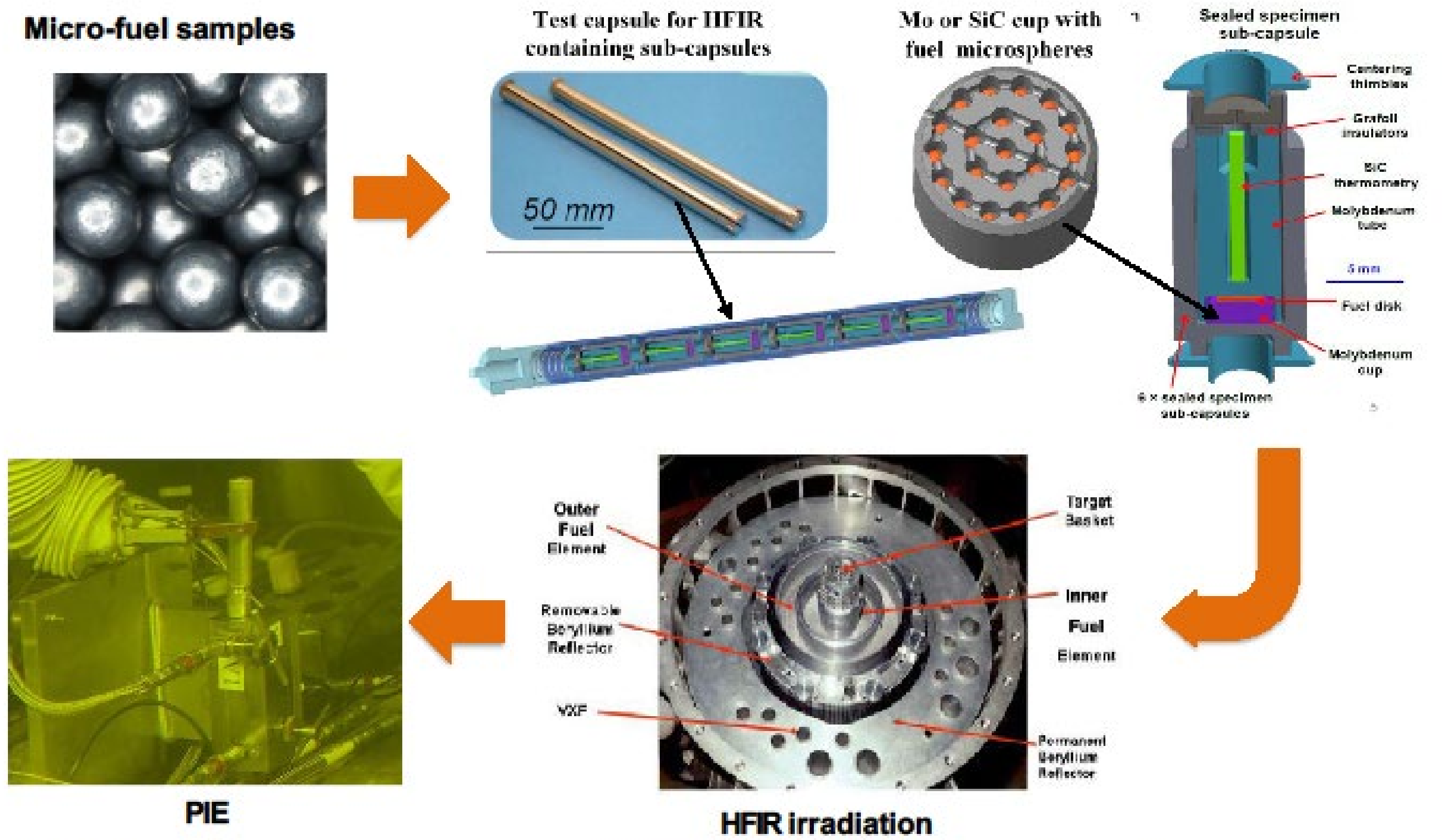
DOE funded project: DE-NE0008819

AFQ Takes Advantage of Modeling and Computer Power Advances



- **Computer extrapolation of sphere behavior to fuel pellet and to fuel rod**

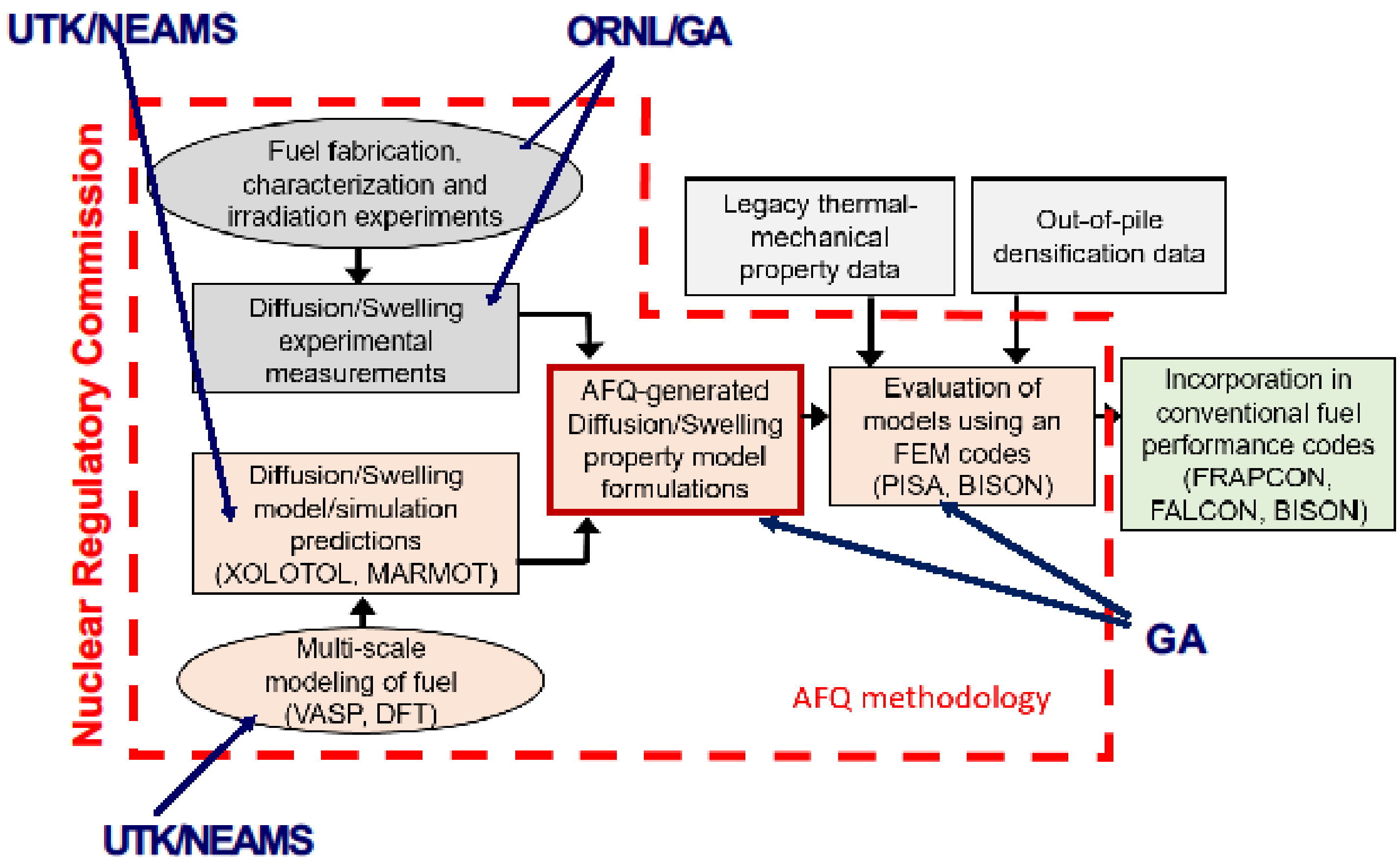
Micro-Capsule Concept Allows Many Test Samples per Irradiation Campaign



7 5/31/19

GENERAL ATOMICS

Multi-Scale Modeling Extrapolates Micro-Fuel Irradiation Results to Fuel Pellet Behavior



NRC Engagement Is Vital: GA's Separate One-Year Pre-Licensing Project as an Example

- Overall licensing plan for use in long-life cores
- SiC/UC testing requirements for demonstration and prototype reactors
- Requirements to validate predictive performance code
- Discuss implementation of AFQ

Project will be implemented through preparation of white papers, review by NRC, and discussion

DOE funded project: DE-NE0008831

9 5/31/19

GENERAL ATOMICS

This AFQ Methodology Is Versatile

This is the first step in the path to realizing AFQ methodology

Next steps:

- The proposed effort demonstrating the AFQ methodology is the first step towards qualifying a new fuel
- This methodology can be further exploited to its full potential as a fast-track qualification process that is equally applicable to any novel fuel concepts

APPENDIX G - Experimental Aspects of Accelerated Fuel Qualification

Experimental Aspects of Accelerated Fuel Qualification

Steven L. Hayes, PhD
Director, Nuclear Fuels and Materials Division

Matthew J. Kerr, PhD
Manager, Nuclear Materials Department

May 31, 2019

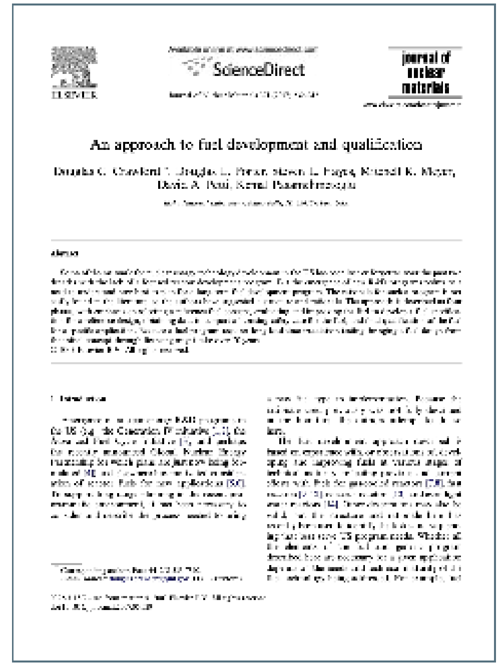
www.inl.gov

Idaho National Laboratory

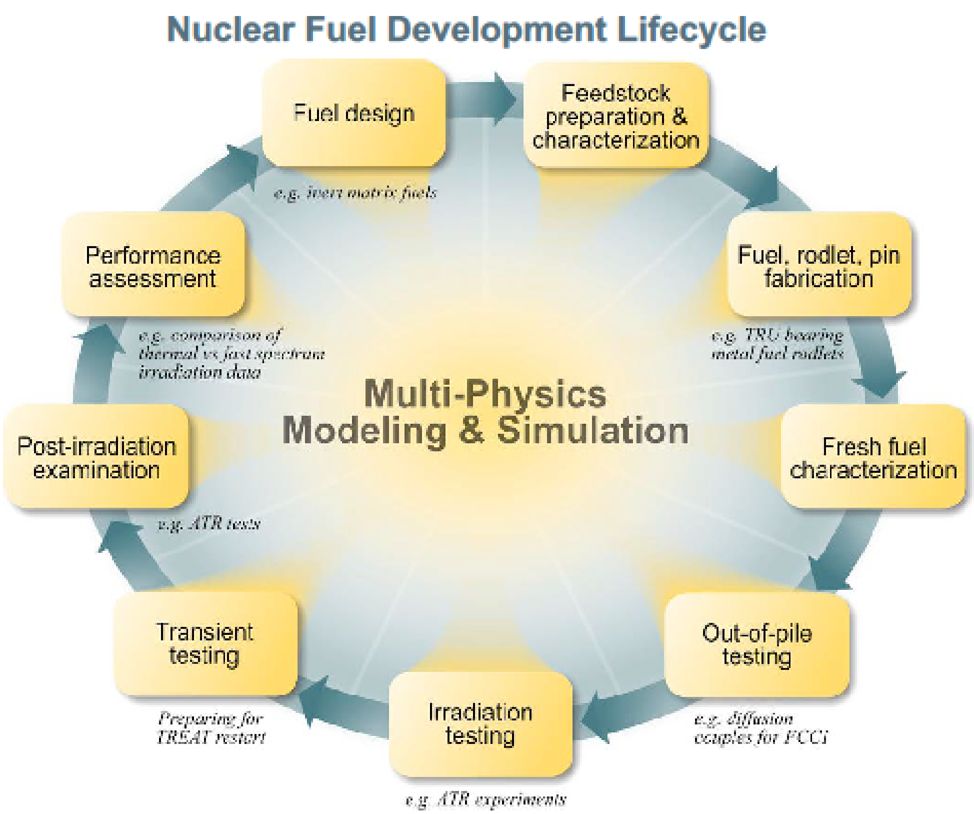
The Challenge of Developing New Fuels

- **Historical Development/Qualification of New Fuels**
  - Most recent review from DOE perspective: ***Journal of Nuclear Materials*, 371** (2007) 232-242
  - Highly empirical in approach
    - Extensive steady-state irradiation testing to optimize fuel design, bound all operating conditions, accumulate adequate statistics, and collect data from (primarily) integral experiments for validation of fuel performance codes
    - Transient testing to bound off-normal and accident scenarios
  - Takes 20-25 years!

- **Urgent Need to Deviate from Historical Paradigm**
  - Testing infrastructure not as extensive as in past
  - Extended timeline discourages innovation and timely deployment of new technologies



Elements of Accelerating the Nuclear Fuel Development Lifecycle



1) Close coupling of experiments and advanced M&S to optimize effectiveness of experiments
2) Separate effects experiments and microstructural characterization to inform and validate mechanistic model development (e.g., MiniFuel rabbits, etc.)
3) Microstructure-based mechanistic fuel modeling, informed/validated using advanced characterization of irradiated fuels and materials at level of microstructure (e.g., **IMCL**)
4) Where appropriate and possible, *in situ* instrumentation of experiments to acquire fuel performance data faster, with insight into path dependence
5) Accelerated integral experiments to validate fuel performance codes (e.g., **FAST**)

2

Microscale Characterization of Irradiated Fuels and Materials

Microstructure-based mechanistic fuel modeling requires characterization of irradiated fuels and materials at level of microstructure for validation.

- IMCL was established to meet this need; gloveboxes provide containment inside shielded enclosures, which house an array of characterization capabilities:
  - Shielded cell for sample preparation
  - Dual beam FIB for preparing TEM lamella, Plasma FIB for preparing block samples for microscale characterization
  - Micro X-Ray Diffraction (µXRD), Electron Probe Micro-Analyzer (EPMA)
  - Laser flash diffusivity, differential scanning calorimetry (DSC), Thermal Conductivity Microscope (TCM)
  - Scanning Electron Microscope (SEM), Transmission Electron Microscope (TEM)

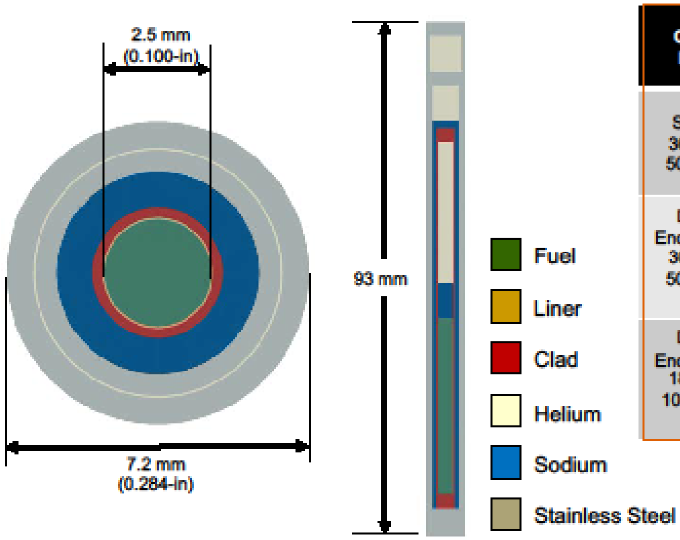
Supports fundamental understanding and additional investment required to support high-throughput experimental campaigns.

Idaho National Laboratory

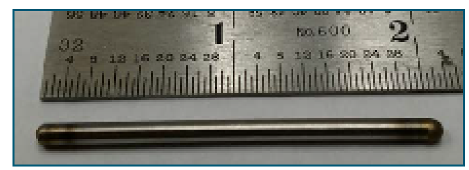
Approach to Accelerated Integral Fuel Testing
(Fission Accelerated Steady-state Testing)

- Revised Capsule Design Objectives:
  1) Increase power density to reduce time to achieve high burnup
  2) Decrease pin diameter to keep peak fuel temperature constant
  3) Reduce sensitivity to fabrication tolerances and capsule/pin eccentricity

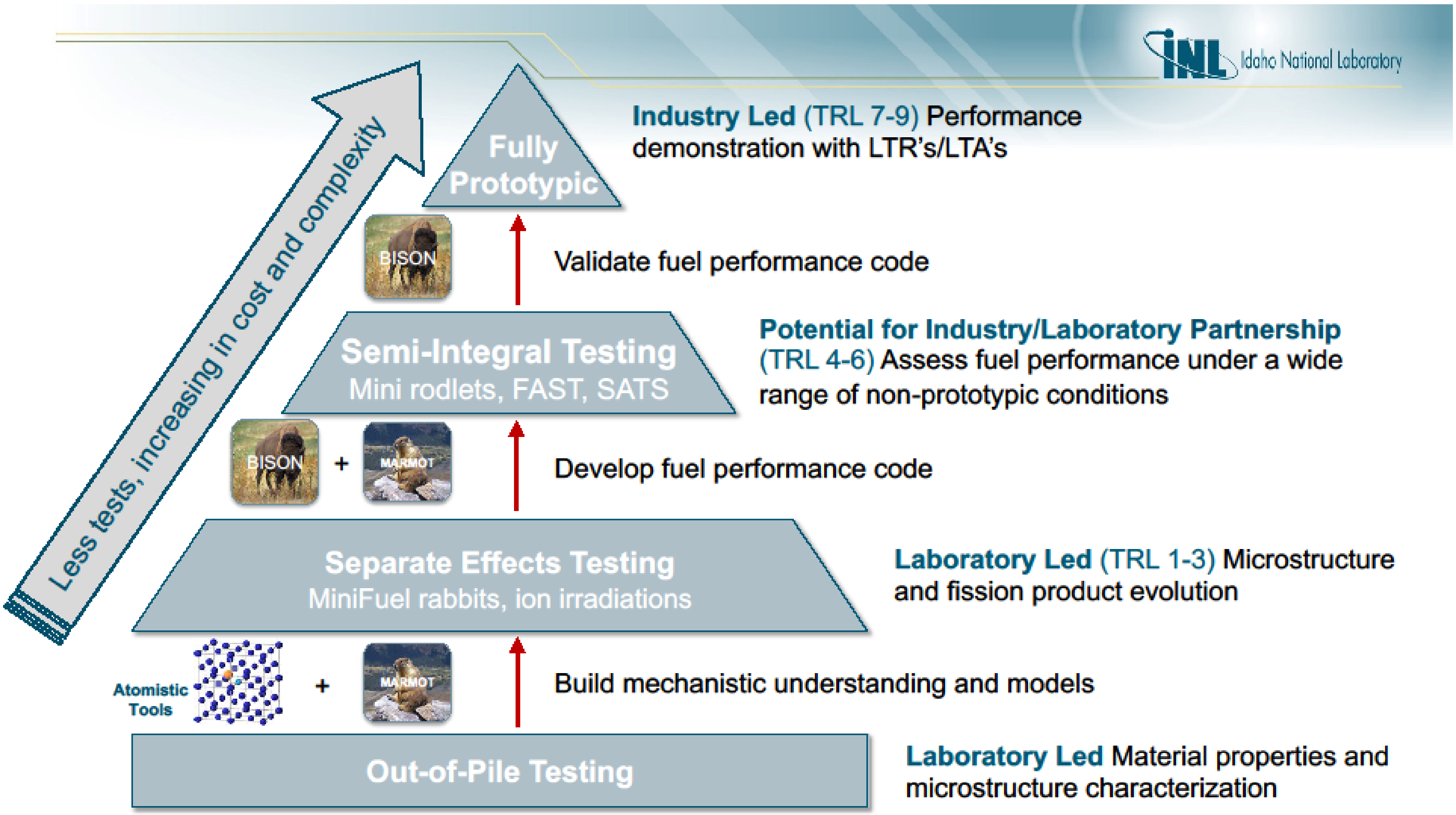
Fabrication trials for 1/2- and 1/3-scale fuel and rodlets is underway



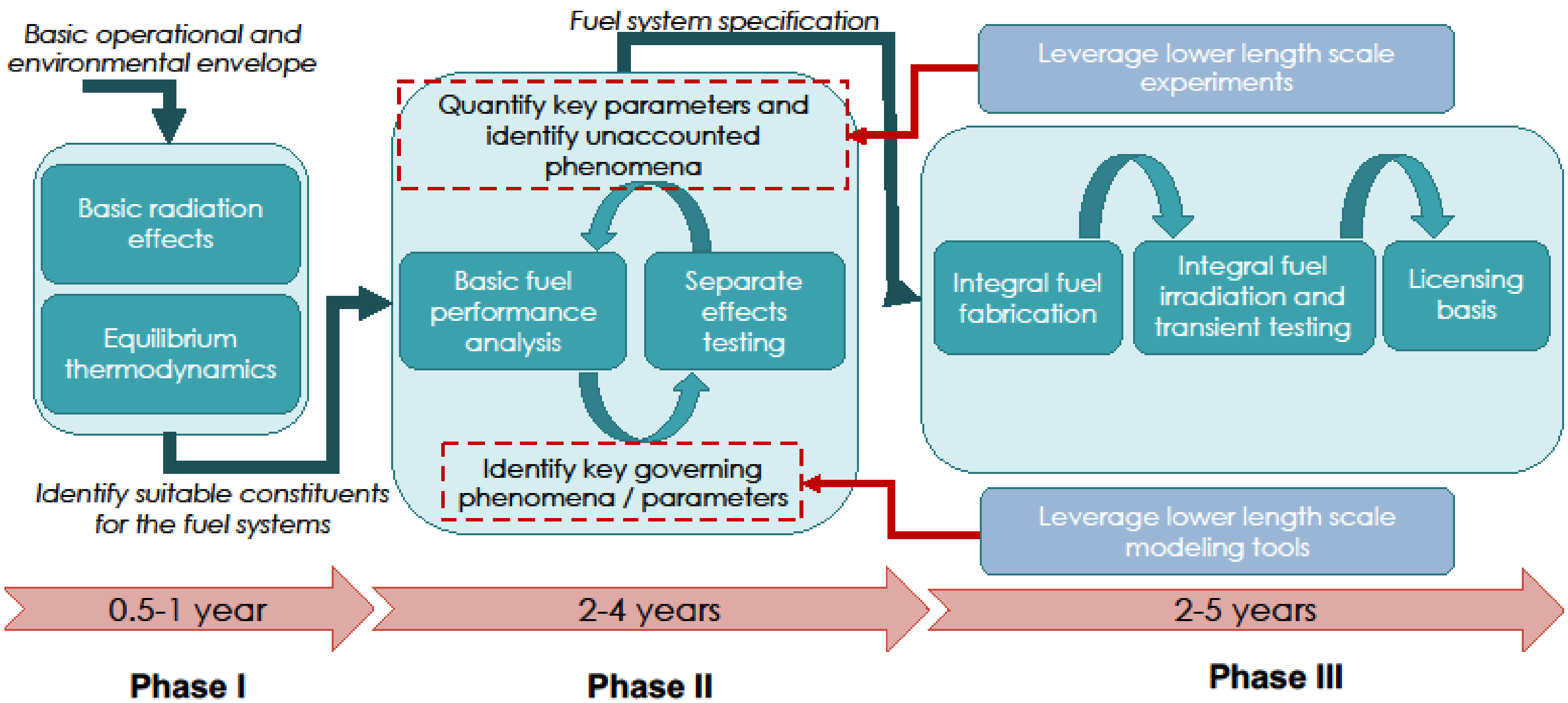
Capsule Design	Cases	Max. Inner Clad Temp (C)	Min. Inner Clad Temp (C)	Peak Fuel Temp (C)
Standard 365 W/cm 50 µm gap	0 µm offset	572	572	709
	25 µm offset	605	483	695
	Difference	+33	-89	-14
Double-Encapsulated 300 W/cm 50 µm gap	0 µm offset	570	570	684
	25 µm offset	567	523	664
	Difference	-3	-47	-20
Double-Encapsulated 180 W/cm 100 µm gap	0 µm offset	566	566	637
	25 µm offset	566	556	629
	Difference	0	-10	-8



One-third diameter pins could achieve >5% burnup/ATR 55-day cycle and reach 30% burnup in less than 2 years.


Idaho National Laboratory
Less tests, increasing in cost and complexity
Fully Prototypic
Industry Led (TRL 7-9) Performance demonstration with LTR's/LTA's
BISON
Validate fuel performance code
Semi-Integral Testing
Mini rodlets, FAST, SATS
Potential for Industry/Laboratory Partnership (TRL 4-6) Assess fuel performance under a wide range of non-prototypic conditions
BISON + MARMOT
Develop fuel performance code
Separate Effects Testing
MiniFuel rabbits, ion irradiations
Laboratory Led (TRL 1-3) Microstructure and fission product evolution
Atomistic Tools + MARMOT
Build mechanistic understanding and models
Out-of-Pile Testing
Laboratory Led Material properties and microstructure characterization

Accelerated approach to fuel qualification



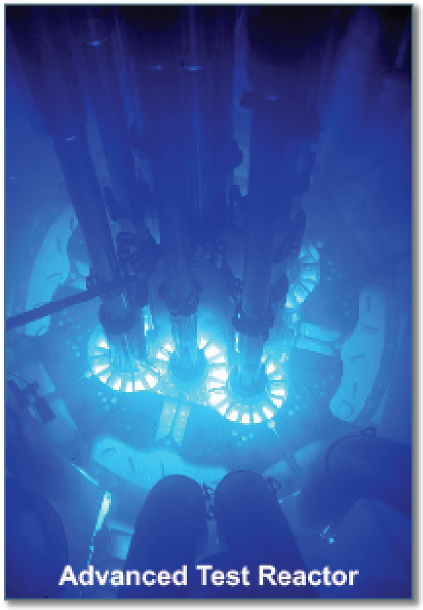
4

Idaho National Laboratory

Summary and Conclusions

- **There is an urgent need to accelerate the development, qualification, and deployment of new fuel systems**
  - Revised DOE perspective is necessary and is in preparation: *An accelerated approach to fuel development and qualification*
- **Advanced M&S has a critical role to play, but experimental aspects of fuel development must also be adapted**
  - More extensive (microstructural) understanding of as-fabricated fuels, as needed input to mechanistic fuel modeling and simulation
  - Postirradiation examinations of fuels and materials that includes microscale characterization, as needed to validate mechanistic models and fuel performance codes
  - New approaches that accelerate irradiation experiments (M&S will need to address the non-prototypicalities introduced by acceleration)
  - Infrastructure investments are likely necessary to support high-throughput experimental campaigns
- **Discussion?**

FIB enclosure in IMCL

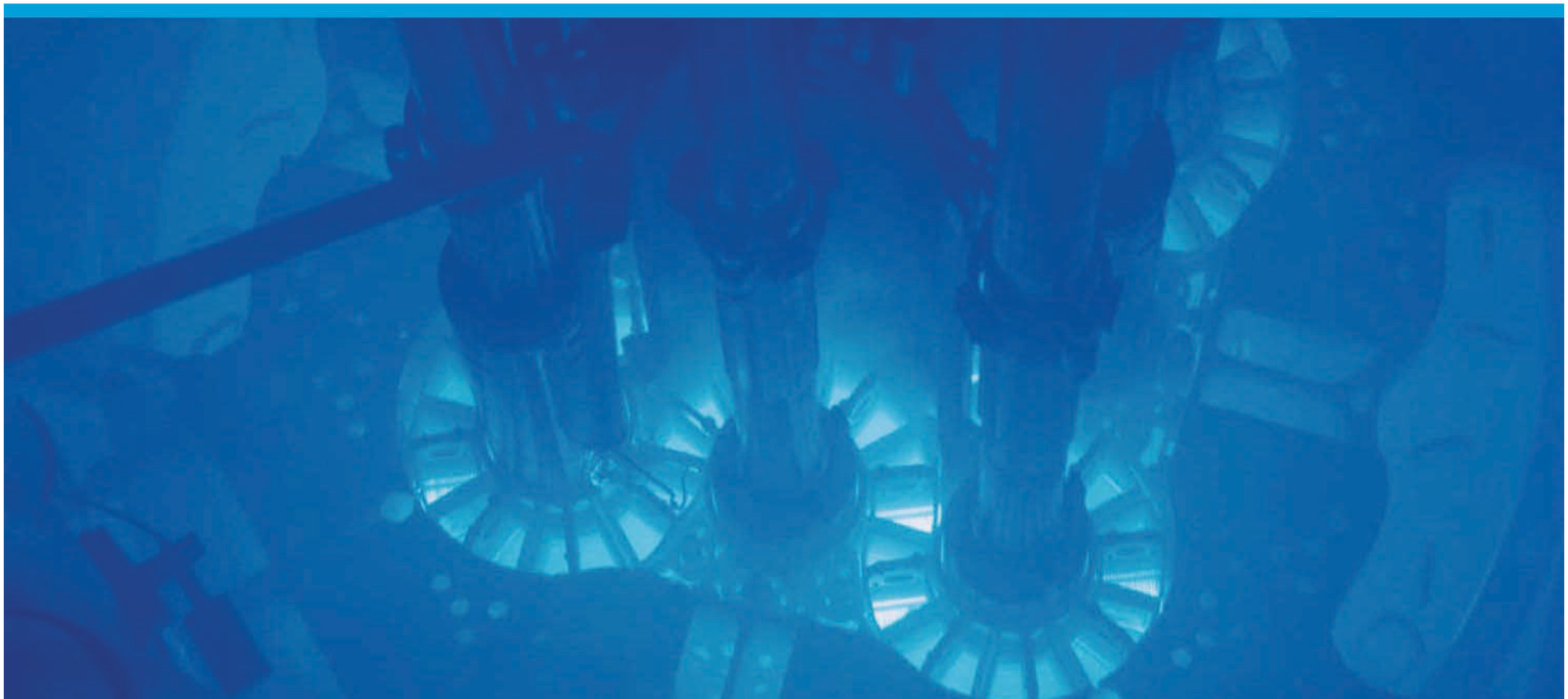


Advanced Test Reactor

APPENDIX H - US DOE-NE Modeling and Simulation

U.S. DEPARTMENT OF ENERGY | Office of NUCLEAR ENERGY

Clean. Reliable. Nuclear.



Christopher Stanek
Los Alamos National Laboratory
NEAMS National Technical Director
stanek@lanl.gov

AFQ Workshop, Washington DC May 31, 2019

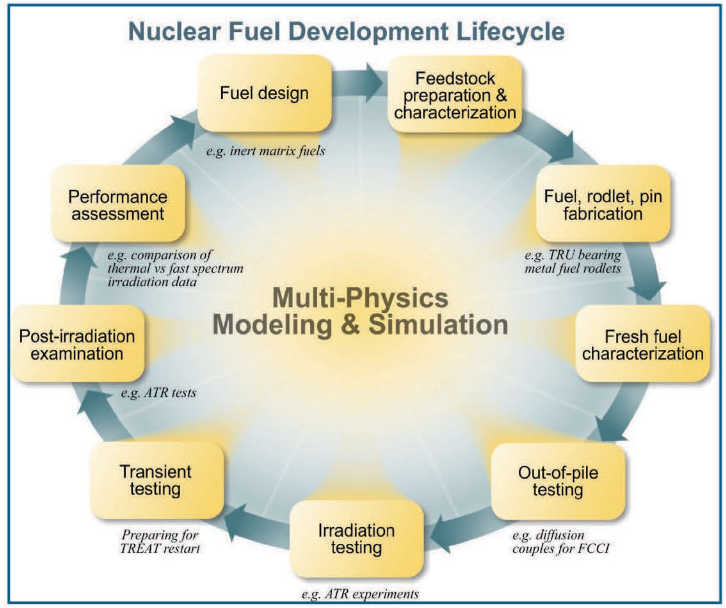
Overview of DOE-NE Mod-Sim in Support of Accelerated Fuel Qualification

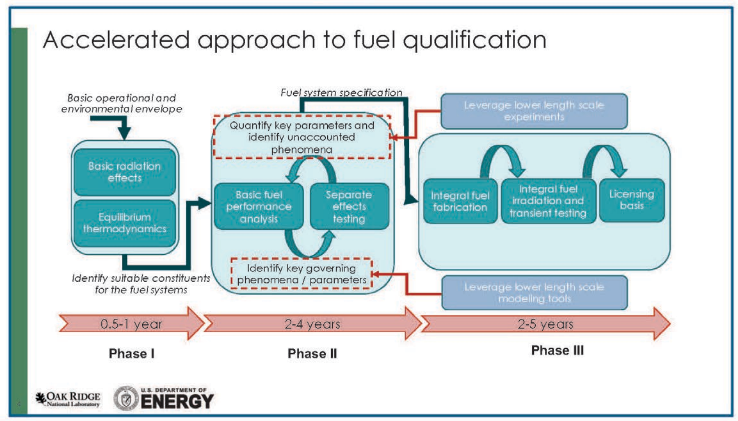
Introduction

At its foundation, AFQ is an inherently non-radical concept. In fact, it is downright conventional to employ mod-sim in conjunction with experiments to solve hard scientific problems.

- *No intention for mod-sim to replace experiments!*
- *Challenge/opportunity is how to employ mod-sim to design more informed experiments or even perform fewer experiments – as well as how to optimally combine mod-sim and experiments.*

Presentation will be an overview of DOE-NE mod-sim programs and several representative examples (extendable to any fuel) in order to stimulate discussion about how to optimally employ mod-sim to accelerate deployment of advanced fuels.



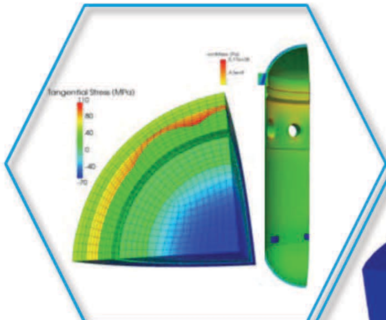


Overview of US DOE-NE Modeling and Simulation

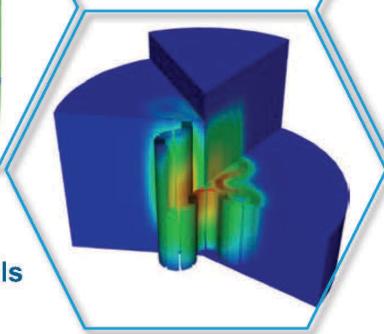
Two significant mod-sim programs:

- Consortium of Advanced Simulation of LWRs (CASL)
- Nuclear Energy Advanced Modeling and Simulation (NEAMS)

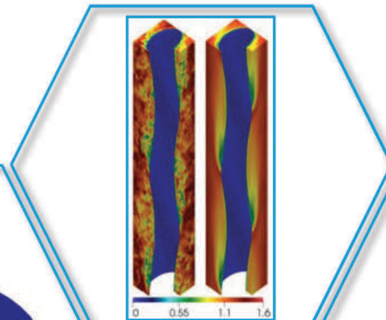
Both programs aim to support accelerated deployment of advanced technologies



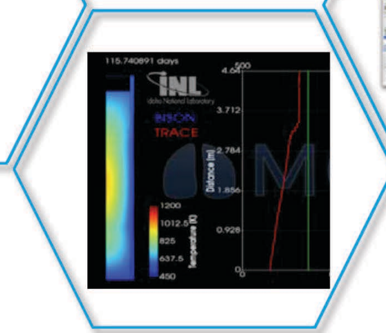
Multiscale fuel performance and structural materials degradation modeling: BISON, GRIZZLY



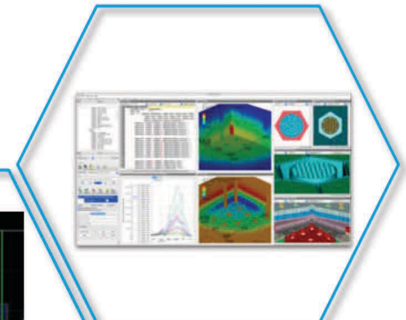
Reactor Physics: PROTEUS, MAMMOTH



Multiscale thermal fluids: SAM, PRONGHORN, Sockeye, Nek5000



Multiphysics: MOOSE



Workflow Management: Workbench

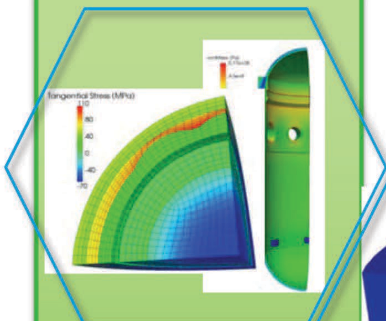
A key priority (and challenge) for DOE-NE mod-sim programs is to strike balance between ***early stage R&D*** and ***industrial relevance***

Overview of US DOE-NE Modeling and Simulation

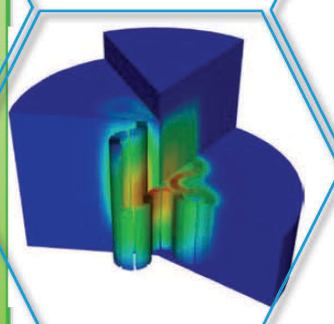
Two significant mod-sim programs:

- Consortium of Advanced Simulation of LWRs (CASL)
- Nuclear Energy Advanced Modeling and Simulation (NEAMS)

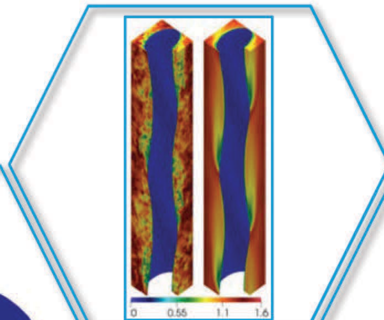
Both programs aim to support accelerated deployment of advanced technologies



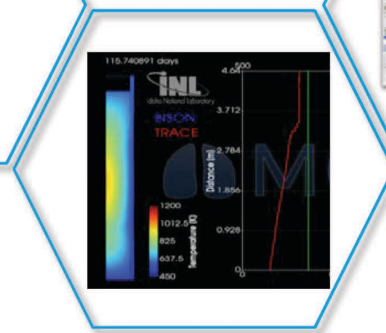
Multiscale fuel performance and structural materials degradation modeling: BISON, GRIZZLY



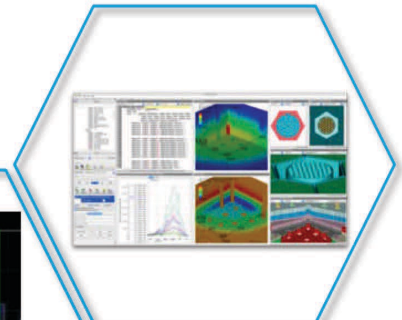
Reactor Physics: PROTEUS, MAMMOTH



Multiscale thermal fluids: SAM, PRONGHORN, Sockeye, Nek5000



Multiphysics: MOOSE



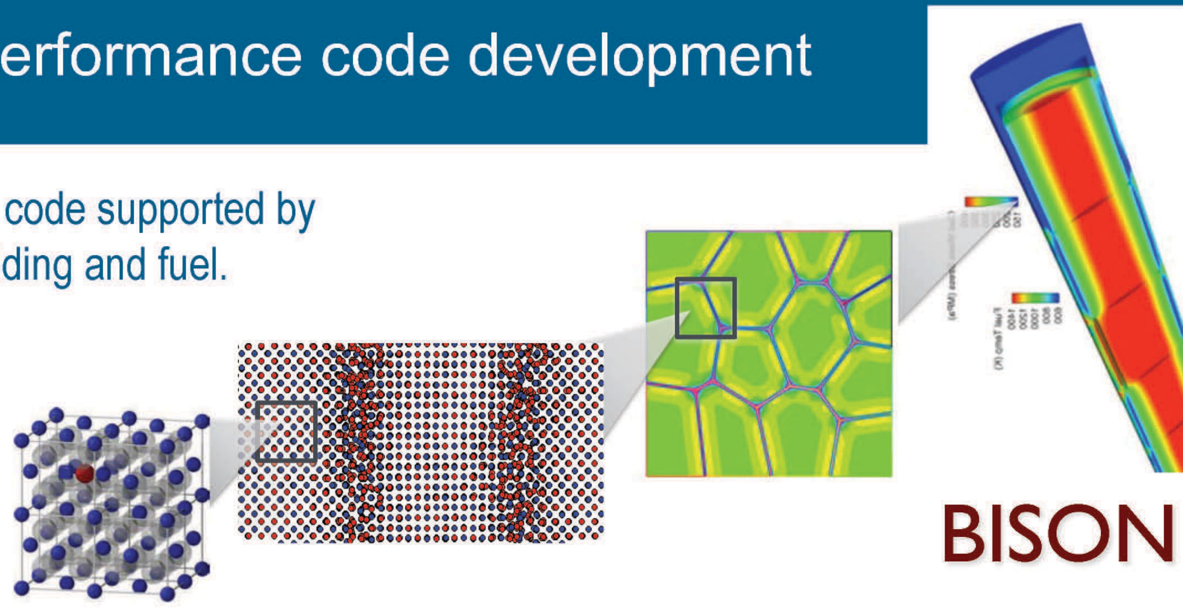
Workflow Management: Workbench

A key priority (and challenge) for DOE-NE mod-sim programs is to strike balance between ***early stage R&D*** and ***industrial relevance***

DOE-NE fuel performance code development

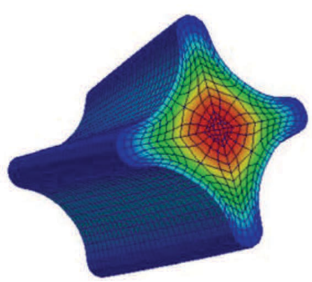
BISON fuel performance code supported by multiscale studies of cladding and fuel.

Insight gained at lower length scales **pragmatically** incorporated in to BISON via constitutive equations, models, parameters, etc.

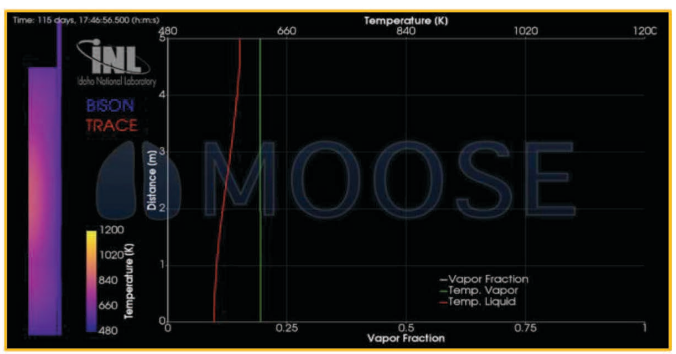


BISON

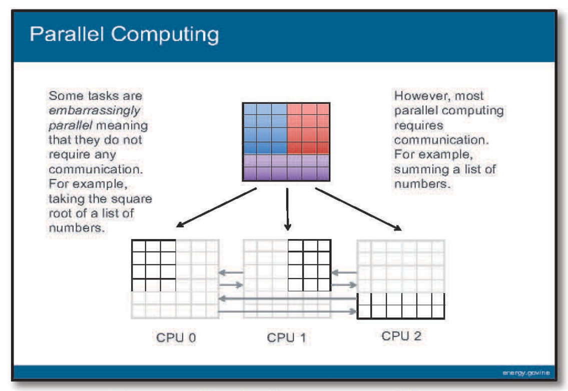
Other key advantages of BISON



3D Fuel Performance



Multiphysics Coupling



Parallel Computing

BISON Software Quality

- MOOSE/**BISON** is supported by >2000 unit and regression tests
- All new code must be supported by verification testing; all tests must pass prior to code merge
- Regularly audited per NQA-1 standards
- Documentation:
  - All tests distributed with source code
  - Code verification process described in journal article

Current view: top level
Test: BISON Test Coverage
Date: 2018-02-07 10:09:49
Legend: Rating: low: < 70 % medium: >= 70 % high: >= 80 %

	Hit	Total	Coverage
Lines:	18111	20668	87.6 %
Functions:	2005	2134	94.0 %

Directory	Line Coverage		Functions	
src	91.7 %	11 / 12	100.0 %	3 / 3
src/actions	88.2 %	903 / 1024	98.1 %	102 / 104
src/auxkernels	83.3 %	992 / 1191	94.6 %	158 / 167
src/auxkernels/tensor_mechanics	87.0 %	40 / 46	100.0 %	5 / 5
src/base	93.5 %	275 / 294	60.0 %	9 / 15
src/bcs	78.3 %	492 / 628	85.5 %	71 / 83
src/bcs/coolant	84.7 %	726 / 857	85.5 %	71 / 83
src/functions	91.9 %	813 / 885	98.2 %	54 / 55
src/ics	99.2 %	130 / 131	100.0 %	5 / 5
src/kernels	80.7 %	630 / 781	87.2 %	136 / 156
src/materials	87.7 %	8268 / 9424	96.2 %	733 / 762
src/materials/tensor_mechanics	91.4 %	2665 / 2915	96.1 %	367 / 382
src/mesh	86.5 %	558 / 645	77.1 %	27 / 35
src/parser	100.0 %	60 / 60	100.0 %	3 / 3
src/postprocessors	91.5 %	668 / 730	94.4 %	151 / 160
src/userobject	83.4 %	818 / 981	94.4 %	101 / 107
src/utils	100.0 %	21 / 21	100.0 %	3 / 3
src/vectorpostprocessors	95.3 %	41 / 43	100.0 %	6 / 6

Annals of Nuclear Energy 71 (2014) 81–90

Contents lists available at ScienceDirect

Annals of Nuclear Energy

journal homepage: www.elsevier.com/locate/anucene

Verification of the BISON fuel performance code

J.D. Hales *, S.R. Novascone, B.W. Spencer, R.L. Williamson, G. Pastore, D.M. Perez

Fuel Modeling and Simulation, Idaho National Laboratory, P.O. Box 1625, Idaho Falls, ID 83415-3840, United States

ARTICLE INFO

Article history:
Received 3 March 2014
Received in revised form 19 March 2014
Accepted 21 March 2014

ABSTRACT

Complex multiphysics simulations such as those used in nuclear fuel performance analysis are composed of many submodels used to describe specific phenomena. These phenomena include, for example, mechanical material constitutive behavior, heat transfer across a gas gap, and mechanical contact. These submodels work in concert to simulate real-world events, like the behavior of a fuel rod in a reactor. If a simulation tool is able to represent real-world behavior, the tool is said to be validated. While much

BISON Validation

- Current assessment status
  - **~75** integral, normal operation and ramp fuel rod experiments
  - **47** LOCA cases (43 burst tests, 4 integral rods)
  - **19** RIA cases
  - Some vendors have performed additional validation w/proprietary data
- Documentation:
  - Assessment report updated annually and distributed with code updates
  - Accessible online
    - User Manual
    - Theory Manual
    - Assessment Report

INL/MIS-13-30314 Rev. 4

September 2017

Assessment of BISON: A Nuclear Fuel Performance Analysis Code

BISON Release 1.4

Idaho National Laboratory
Fuel Modeling and Simulation Department
Idaho Falls, Idaho 83415

https://bison.inl.gov/SiteAssets/BISON_assessment1.4.pdf

Nuclear Engineering and Design 301 (2016) 232–244

Contents lists available at ScienceDirect

Nuclear Engineering and Design

journal homepage: www.elsevier.com/locate/nucengdes

Validating the BISON fuel performance code to integral LWR experiments

R.L. Williamson[a,*], K.A. Gamble[a], D.M. Perez[a], S.R. Novascone[a], G. Pastore[a], R.J. Gardner[a], J.D. Hales[a], W. Liu[b], A. Mai[b]

[a] Fuel Modeling and Simulation, Idaho National Laboratory, P.O. Box 1625, Idaho Falls, ID 83415-3840, United States
[b] ANATECH Corporation, 5435 Oberlin Dr., San Diego, CA 92121, United States

HIGHLIGHTS

- The BISON multidimensional fuel performance code is being validated to integral LWR experiments.
- Code and solution verification are necessary prerequisites to validation.
- Fuel centerline temperature comparisons through all phases of fuel life are very reasonable.
- Accuracy in predicting fission gas release is consistent with state-of-the-art modeling and the involved uncertainties.

Case Study 1:
3D Fuel Performance

N. Capps, et al., “Evaluation of missing pellet surface geometry on cladding stress distribution and magnitude,” *Nucl, Eng. Design* **305** (2016) 51.

Many different potential use cases for BISON fuel performance code – though our efforts intentionally avoid duplicating capability.

Certain 3D fuel concerns lend themselves to BISON, e.g. missing pellet surface, where thermomechanical response be accurately simulated.

Several advanced fuel designs have 3D features that can be simulated with BISON.

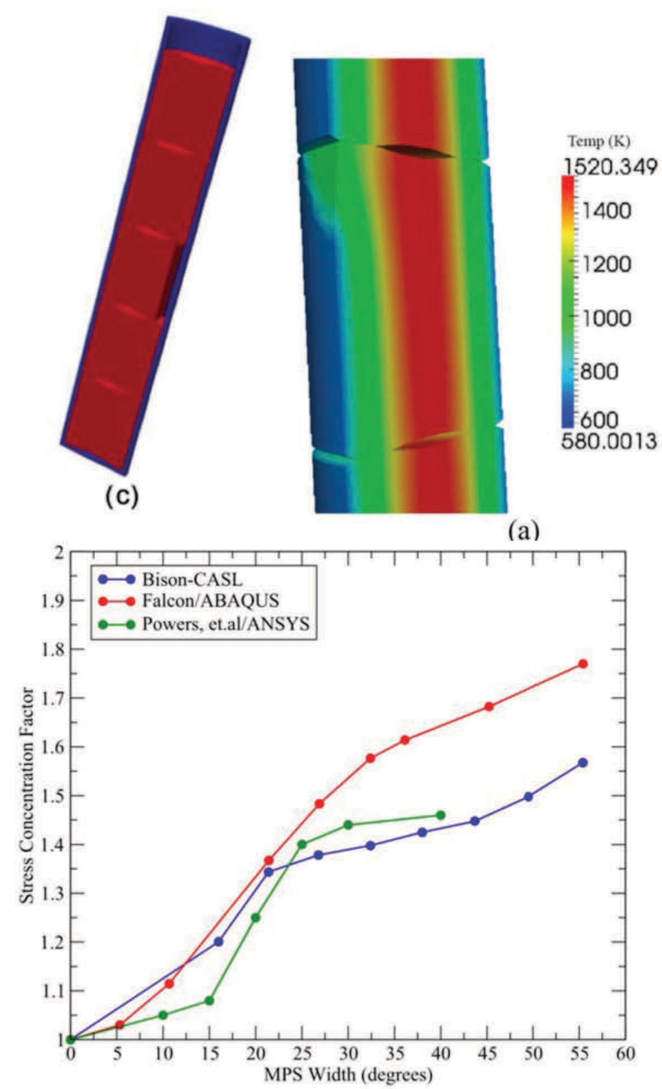
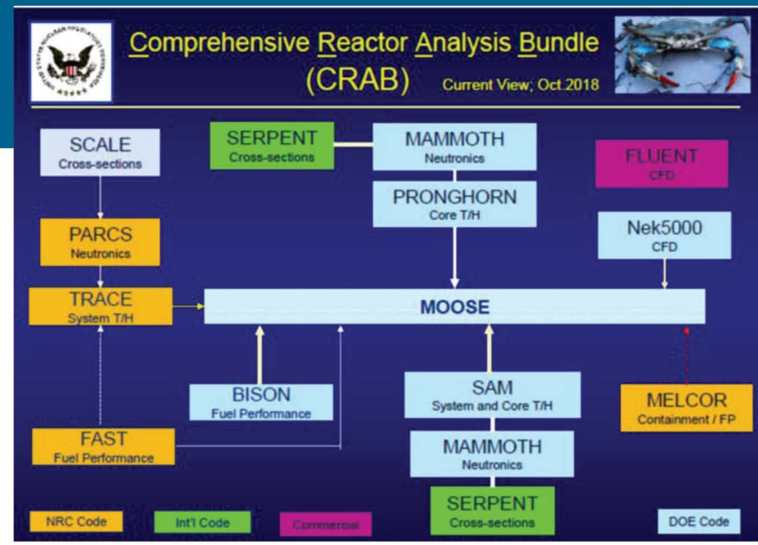


Fig. 19. 3-D Bison-CASL stress concentration factor, as a function of MPS defect width, compared to values from literature (Roberts and Gelhaus, 1979; Lansiart and Michel, 2009).

Case Study 2:
Multiphysics Feedback

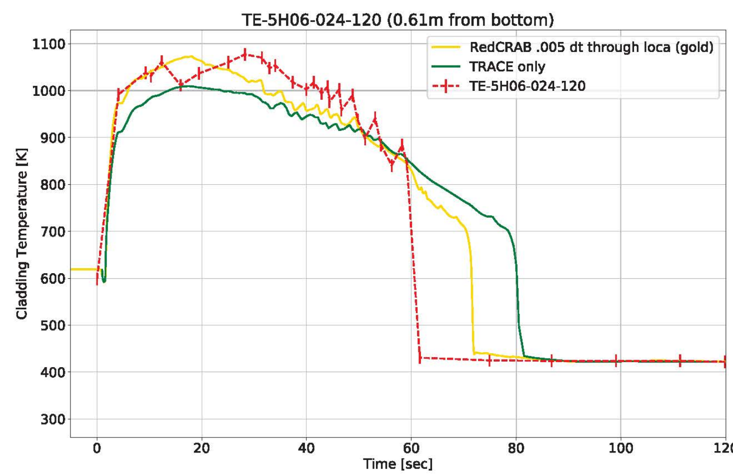


slide courtesy of Steve Bajorek (RES) – and from "NRC Non-Light Water Reactor (Non-LWR) Vision and Strategy, Volume 1 – Computer Code Suite for Non-LWR Design Basis Event Analysis" (ML19093B322)

For non-LWRs, NRC has proposed to use BISON for design basis event analysis within CRAB suite (ML19093B322). Additional fuel performance specific report for non-LWRs pending.

Coupling has been established between TRACE (system thermal hydraulics) and BISON via nonlinear heat transfer coefficients.

Initial TRACE-BISON results of cladding T for LOFT L2-5 demonstrate improved agreement with experiment compared to standalone TRACE. Work is ongoing to improve quench front resolution. Preliminary FeCrAl calculations underway.



Case Study 3+n:

Using computational materials science to inform BISON

Why fission gas?: Difficult to asses experimentally, not much data for new fuels, important implications for fuel performance.

Current empirical FG diffusion model for UO_2:

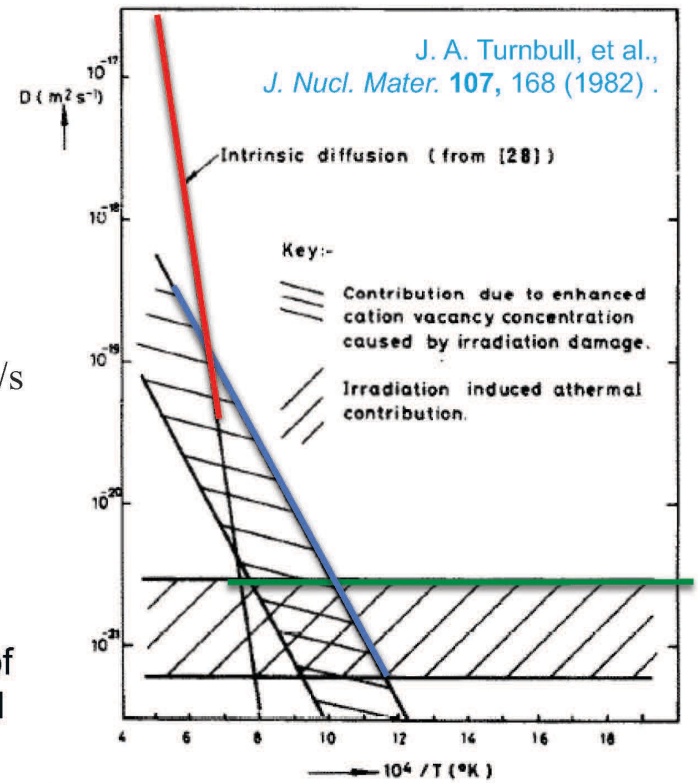
Total: $D_{Xe}=D_1+D_2+D_3$

Intrinsic: $D_1 = 7.6\cdot 10^{-10} \times \exp\left(-\frac{3.04}{k_B T}\right) \mathrm{m}^2/\mathrm{s}$

Irr. Enhanced: $D_2 = 4\times 1.41\cdot 10^{-25} \times \sqrt{\dot{F}} \exp\left(-\frac{1.20}{k_B T}\right) \mathrm{m}^2/\mathrm{s}$

Athermal: $D_3 = 4\times 2\cdot 10^{-40} \times \dot{F}\ \mathrm{m}^2/\mathrm{s}$

- The mechanisms for D_1, D_2 and D_3 are not fully understood, which complicates development of predictive models.
- D_1 and D_2 obtained from a reaction-diffusion model of defect evolution parameterized by DFT and empirical potential calculations.
- D_3 from direct molecular dynamics cascade and thermal spike simulations.



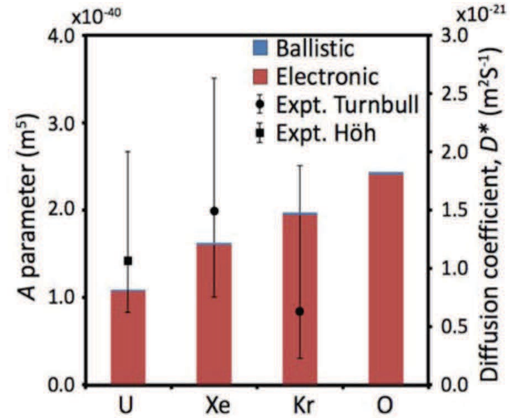
Similar data does not exist for other advanced fuel designs. Therefore employ atomistics to develop fission gas diffusion model.

Athermal fission gas diffusion and resolution

W Setyawan, MWD Cooper, ..., BD Wirth, *J. Appl. Phys.* **124** (2018) 075107.
M.W.D. Cooper, et al. *J. Nucl. Mater.* **481** (2016) 125
M.W.D. Cooper, et al. *J. Phys. Cond. Matter,* **28** (2016) 405401

SciDAC Scientific Discovery through Advanced Computing — Office of Science

Thorough molecular dynamics simulations (thermal spike and radiation damage cascade) have revealed underlying mechanisms governing D_3 and resolution in UO_2, e.g. electronic component dominates D_3.



Mechanistic model developed for resolution (below), which is in good agreement with previous (Turnbull and Lösönen) empirical models :

Turnbull's model of re-solution rate:

$$b_{het} \equiv \underbrace{\pi(R_b + R_f)^2}_{\text{area of influence}}(2\underbrace{\dot{F}}_{\text{fission rate density}}\underbrace{\mu_f}_{\text{range of fission gas}}) \text{ (completely re-solved)} \quad \approx 1.5 \times 10^{-3} \text{ /s}$$

$R_b = R_f = 1$ nm
$\dot{F} = 10^{-8}$ nm^{-3}s^{-1}
$\mu_f = 6$ μm

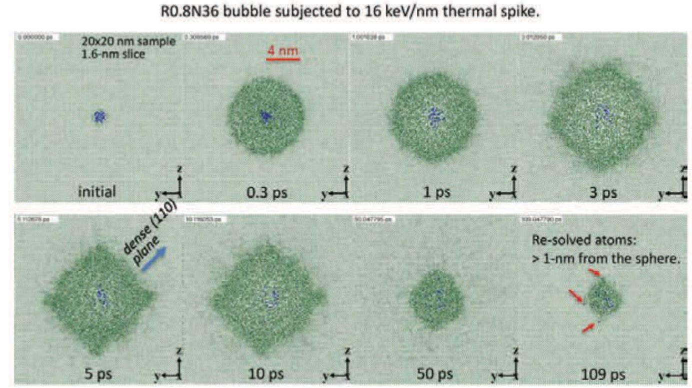
Should be modified to:

$$b_{het} \equiv \pi(R_b + R_f)^2(2\dot{F}\mu_f) * 0.25\{1 - exp[-0.1967(S_{eff} - 9.042)e^{-1.1756Rb}]\}$$

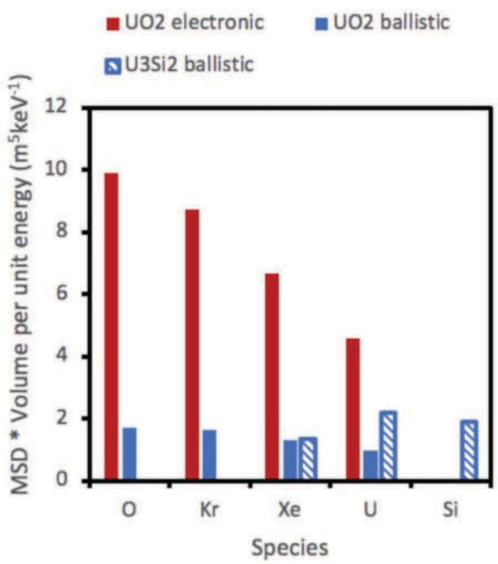
$$b_{het} \equiv \pi(R_b + R_f)^2(2\dot{F}\mu_f) * \frac{1}{\mu_f}\int_0^{\mu_f} 0.25\{1 - exp[-0.1967(\underbrace{S_{eff}}_{\text{depend on x}} - 9.042)e^{-1.1756Rb}]\}dx$$

for $S_{eff} > 9.042$ keV/nm, else the integrant = 0.

R0.8N36 bubble subjected to 16 keV/nm thermal spike.



D_3 prediction for U_3Si_2



White *et al.*, *J. Nucl. Mater.* **464** 275-280 (2015)

U_3Si_2 thermal conductivity

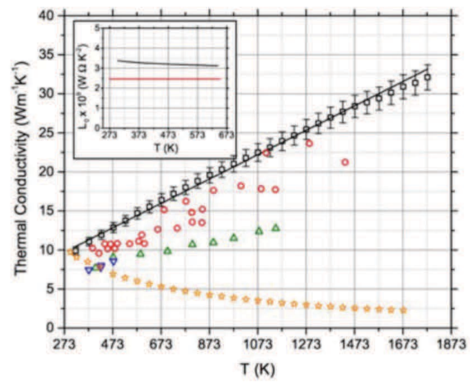
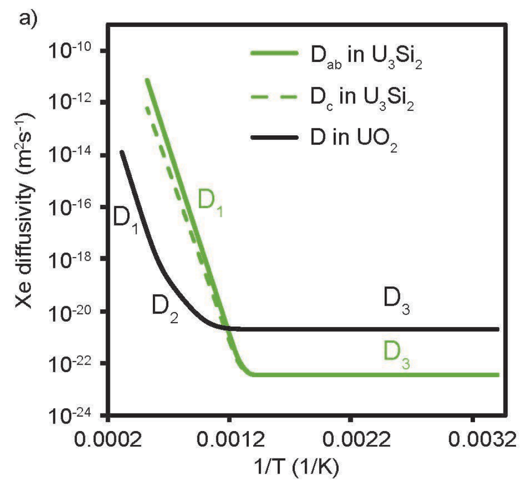


Fig. 6. Calculated thermal conductivity data for U_3Si_2 as a function of temperature to 1773 K collected in this study (□). Reference data from Shimizu [17] is represented by (○), (▽), and (△). Literature values for UO_2 (☆) are included from [26]. An inset is provided to compare the expected Lorenz values (—) with calculated values (—).

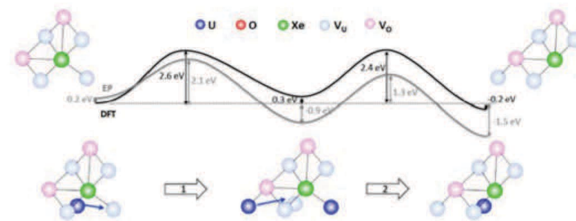


- Similar displacement per unit energy deposited via ballistic stopping as for UO_2.
- High thermal conductivity of U_3Si_2 dissipates heat in thermal spike so quickly that no displacement occurs.
- Most fission fragment energy is still deposited electronically but does not create diffusion (unlike in UO_2).

D_3 predicted to be two orders of magnitude slower in U_3Si_2 than UO_2.

Models for D_1 and D_2 in undoped UO_2

- A cluster dynamics model (Matthews et al. under review), based on DFT description of defect energetics, solves a set of coupled rate equations to describe:
  - Source term for interstitials and vacancies (irradiation)
  - Annihilation of defects
  - Clustering of defects
  - Separation of clusters to smaller clusters and point defects
  - Sink terms for all clusters and point defects
  - O defects treated in equilibrium
- Provides a quantitative description of both the D_1 and D_2 Xe diffusion regimes
- Demonstrates the role of enhanced point defect concentrations in stabilizing the large/mobile defect clusters



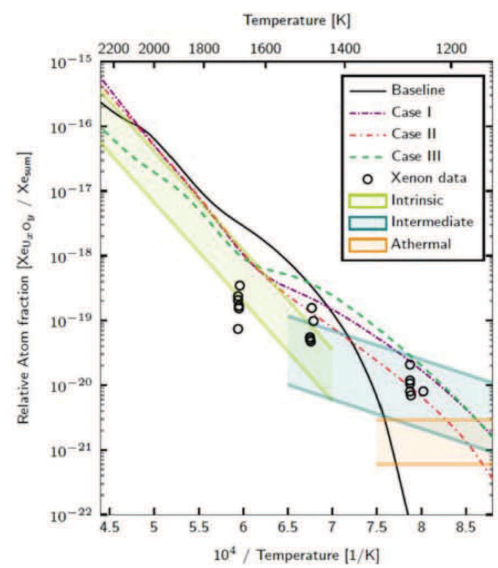
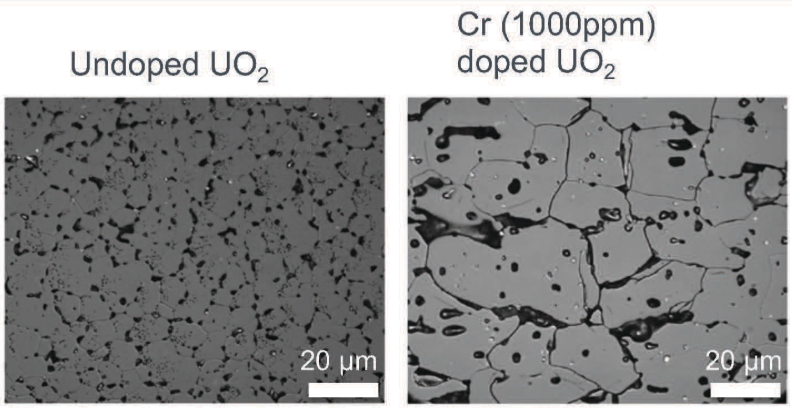


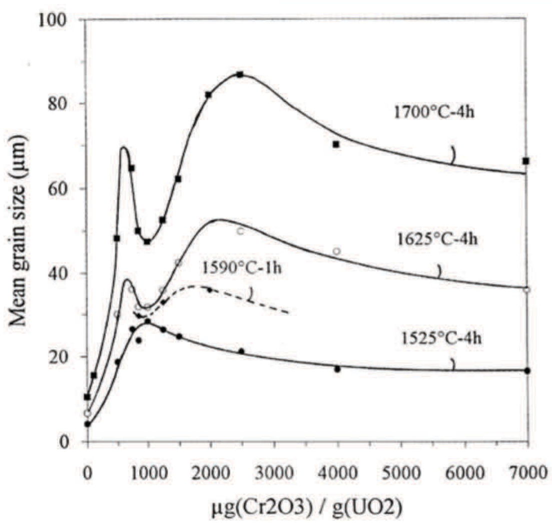
Figure 13: Xenon diffusivity for several different cases: Baseline (values from Appendix B), the "best case" for uranium self-diffusion from Case I from Matthews et al. [12] ($Q_{V_U} \times 0.9$, $H_{O_i} = -0.51$ eV, $H_{P_{O_2}} = 5.5$ eV), Case II (same as Case I with $H_{P_{O_2}} = 5.1$ eV), and Case III (same as Case II with $T_0 = 1773$ K).

D. A. Andersson, et al., J. Nucl. Mater. **451**, 225 (2014).
D. A. Andersson, et al., Phys. Rev. **84**, 054105 (2011).
D. A. Andersson, et al., J. Nucl. Mater. **462**, 15 (2015).

Fission Gas Release in doped-UO_2



Aborelius *et al. J. Nucl. Sci. Tech.* **43** 967-976 (2006)



Bourgeois *et al. J. Nucl. Mater.* **297** 313-326 (2001)

Cr-doped UO_2 exhibits larger grains than undoped (4-5 times w/ 1000 ppm Cr)

Mechanism is somewhat unclear: *liquid phase sintering vs. solid state defect (cation) transport.*

Two important potential implications of this study. Rigorous understanding of Cr defect physics will permit:
(1) optimized doping procedures.

(2) development of predictive fuel performance models (e.g. fission gas release).

NEAMS
NUCLEAR ENERGY ADVANCED MODELING & SIMULATION PROGRAM

Uranium defects are key to enhanced mass transport and sintering

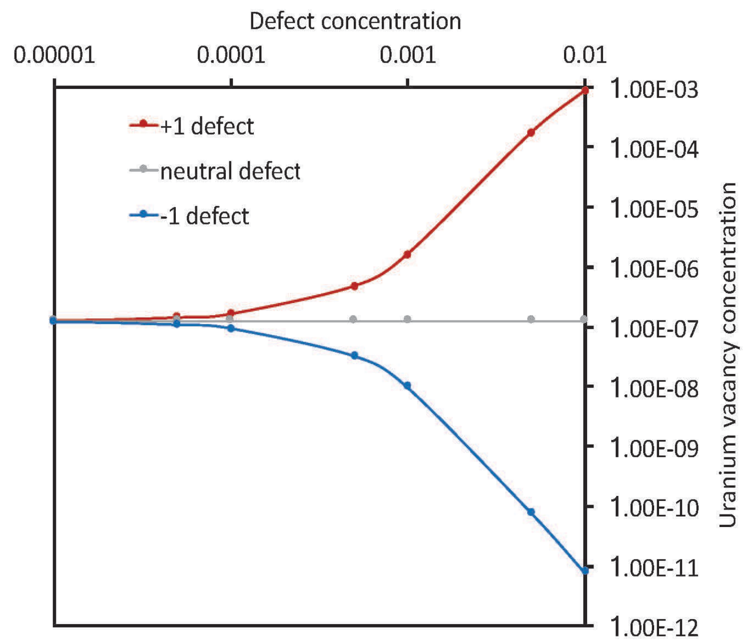
- U vacancy concentrations are key to U mass transport
- U vacancies are negatively charged defects
- If Cr solution occurs via a negative defect (e.g. Cr^{3+} substituting for U^{4+}), then U vacancy concentration is suppressed
- If Cr solution occurs via a positive defect (e.g. interstitial), then U vacancy concentration is enhanced.

Options =

Cr_U' Cr_U'' *Net negative*

$Cr_U^{\times}$ *Charge neutral*

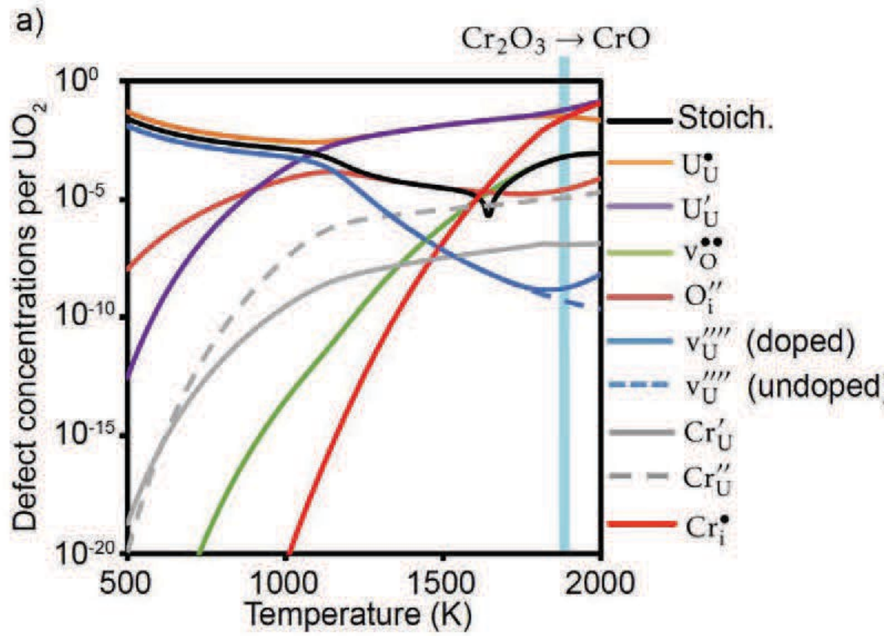
$Cr_U^{\bullet\bullet}$ $Cr_U^{\bullet}$ $Cr_i^{\bullet\bullet\bullet}$ $Cr_i^{\bullet}$ $Cr_i^{\bullet\bullet\bullet\bullet\bullet}$ $Cr_i^{\bullet\bullet}$ $Cr_i^{\bullet\bullet\bullet\bullet}$ $Cr_i^{\bullet\bullet\bullet\bullet\bullet\bullet}$ *Net positive*



Uranium defects also govern fission gas diffusion. So any effect of dopant on sintering kinetics will also impact FG diffusivity.

Cr-doped UO_2 Results

- DFT results indicate that at low temperatures very low Cr solubility at substitutional sites
  - Cr forms a negative defect at substitutional sites but negligible concentrations
- At high temperature vibrational entropy drives solubility onto the interstitial site
  - Significant concentrations of 1+ interstitial at sintering temperatures (>1700 K)
- Outer shell has 5 *d* electrons allowing multiple valence states



M.W.D. Cooper, C.R. Stanek and D.A. Andersson, "The role of dopant charge state on defect chemistry and grain growth of doped UO_2," *Acta Materialia* **150** (2018) 403.

Limiting consideration to Cr^{3+} or ignoring vibrational entropy will not capture role of Cr-doping

Doped UO_2 Fission Gas Behavior

Killeen, *JNM* 88 (1980) 177.

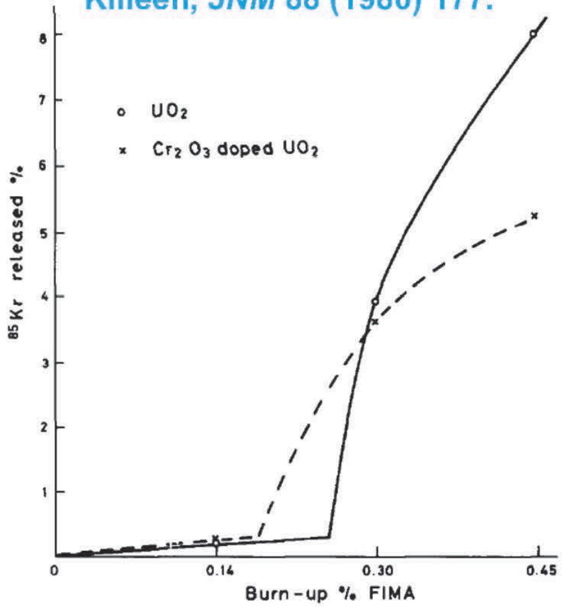


Fig. 2. Plot of gas release against burn-up. The curves are plotted from eq. (2) for the undoped samples and eq. (4) for the doped samples. The release values shown here have been corrected as described in the text to allow for evaporation loss and temperature differences between the samples.

$$D^{UO_2}\,(1465°C) = 1.3 \times 10^{-20}\ m^2/s\ ,$$

$$D^{Cr_2O_3}\,(1500°C) = 7.9 \times 10^{-20}\ m^2/s\ ,$$

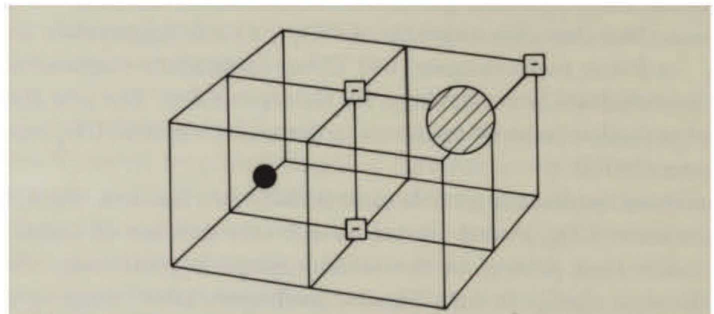


FIGURE 8. Complex of impurity, gas atom and anion vacancies. ●, Impurity atom at vacant cation site.

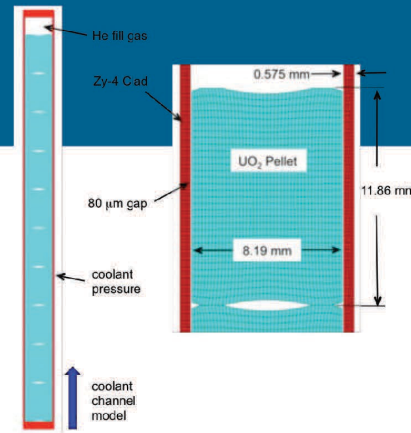
CRA Catlow, *Proc Roy Soc A* **364** (1978) 473.

Previous explanation (40 years ago!), relying on diffusion of large clusters, is likely inaccurate.

Grains ~5x larger but diffusivity ~5x faster for doped-UO_2. Fuel performance calculations to closely examine effect.

NEAMS
NUCLEAR ENERGY ADVANCED MODELING & SIMULATION PROGRAM

Initial BISON Test Cases

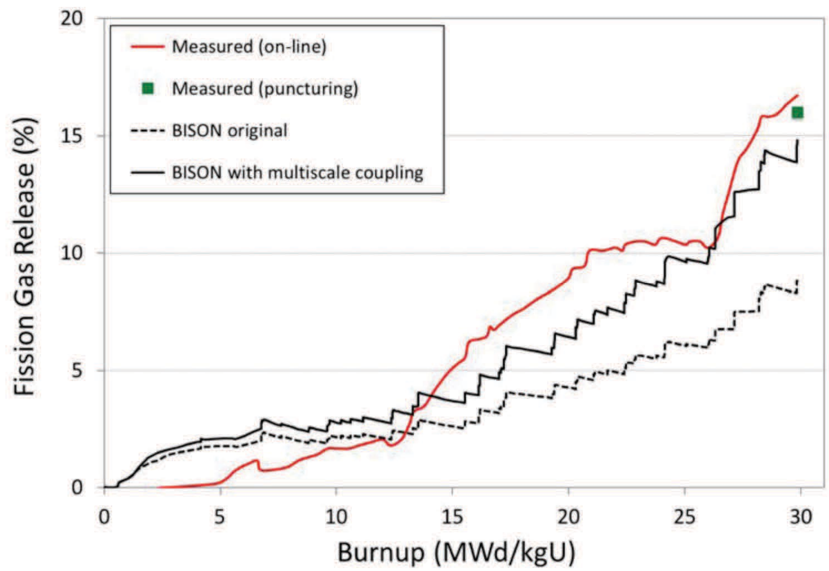


Recent results of Giovanni Pastore (INL)

BISON simulations of Halden 677 (rod 5) comparing existing empirical BISON FG model (factor 3 correction from undoped UO_2) with atomistically-informed (and temperature dependent) doped-UO_2 diffusivity model.

Physics-based multiscale model better reproduces experimental data than does empirical correction.

Clear demonstration of a functional multiscale fuel performance model that serves as a foundation for extension to other advanced fuel types.



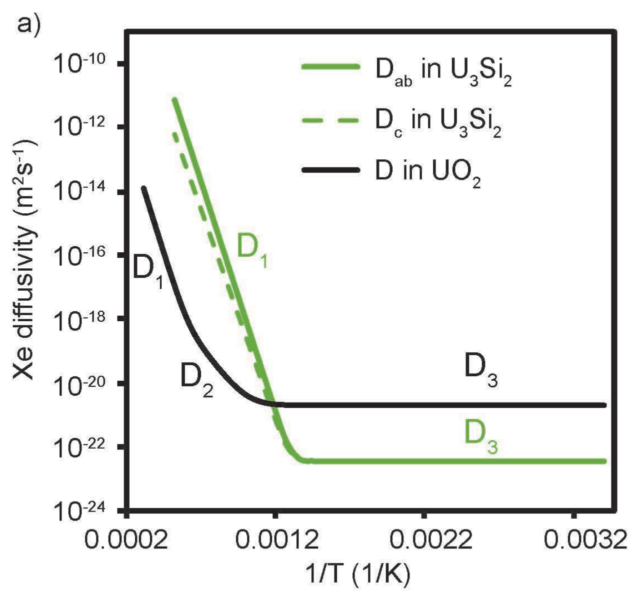
**Tech Rep. HWR-872, OECD Halden Reactor Project, 2008*

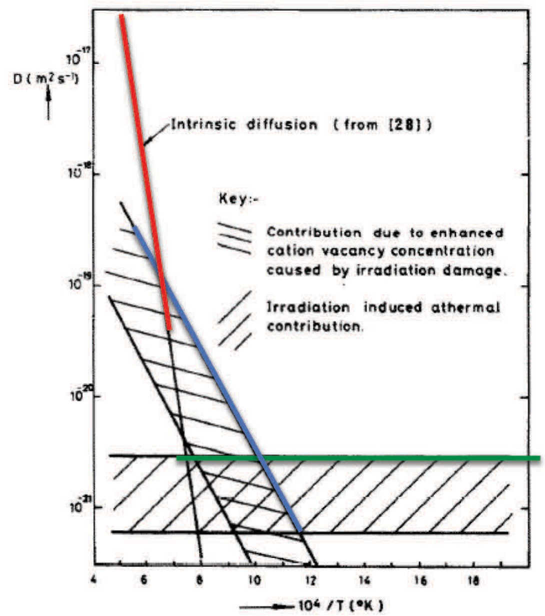
D_1 fission gas diffusion in $U_3Si_{2\pm x}$

Andersson, Liu, Beeler, Middleburgh, Claisse, Stanek, *J. Nucl. Mater.* **337** 271-278 (2018)

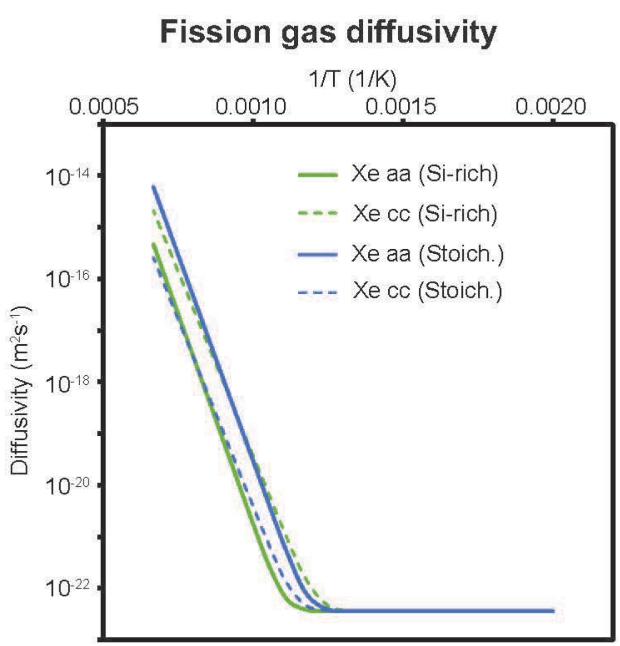
DFT employed to describe intrinsic (thermal) diffusion.

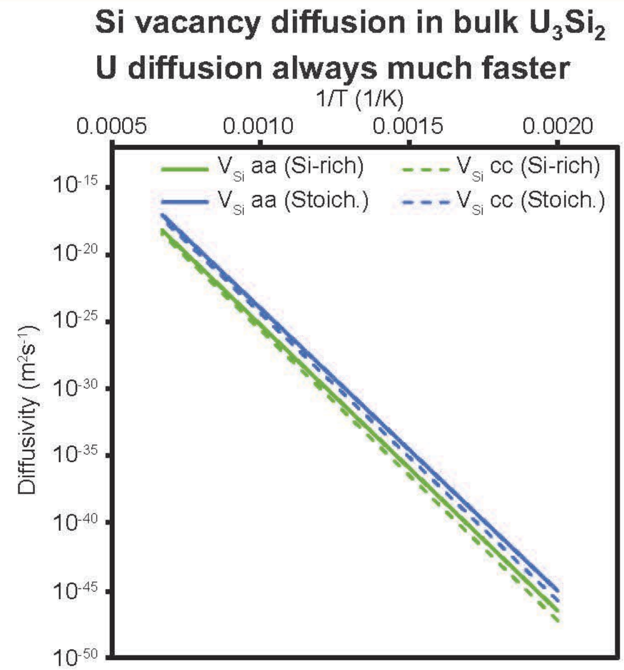
Implication for U_3Si_2 FG diffusion w.r.t. UO_2: Lower athermal diffusivity (D_3) in U_3Si_2 (compared to UO_2) but higher intrinsic diffusivity (D_1).





U_3Si_2: Stoichiometry dependence and vacancy behavior



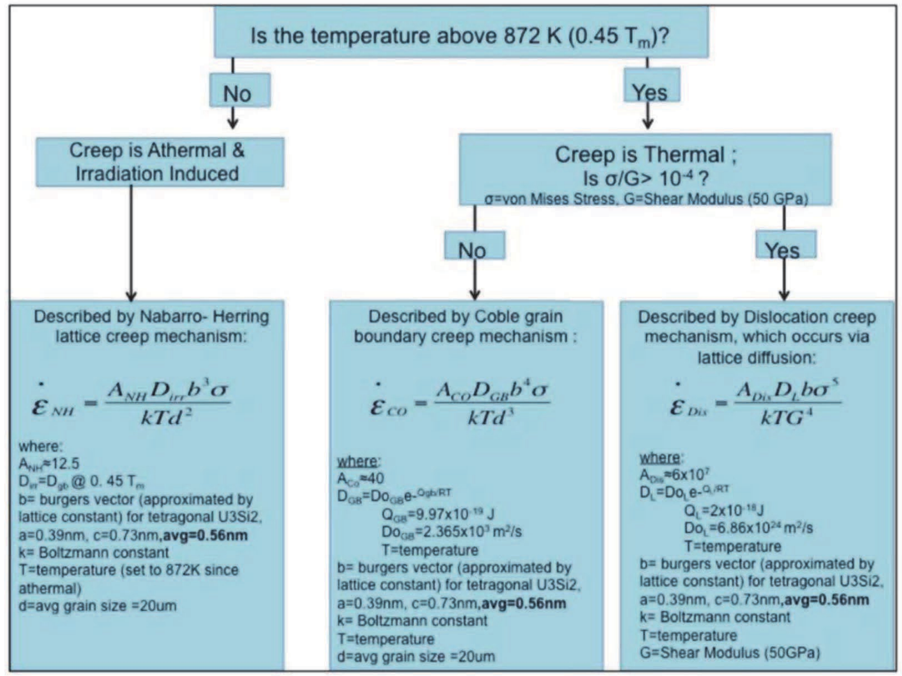


- Fission gas diffusion was calculated for D_1 using DFT and D_3 using molecular dynamics
  - Updated equations passed to longer length/timescale models
- Si vacancy diffusion was shown to be much lower than U vacancy diffusion and is therefore limiting for void and bubble growth
  - Updated equations passed to mesoscale and engineering scale simulations
- Ongoing work to develop a cluster dynamics model for capturing irradiation effects on both fission gas and point defect diffusion

Optimizing complex engineering models

- As physics insight is accumulated, it is often the case that the information can be applied to different fuel performance problems.
- Work is underway, using Metzger fuel creep model as a framework, to provide specific parameters that are sources of uncertainty in BISON.
- Similar examples exist for metallic fuel swelling, which is an aggregate effect of a number of different phenomena

U_3Si_2 creep model, developed by Metzger for BISON



Summary

Representative results presented for how relatively fundamental studies can be employed to address engineering scale analysis and contribute to accelerated fuel qualification. (Similar results for cladding not shown today)

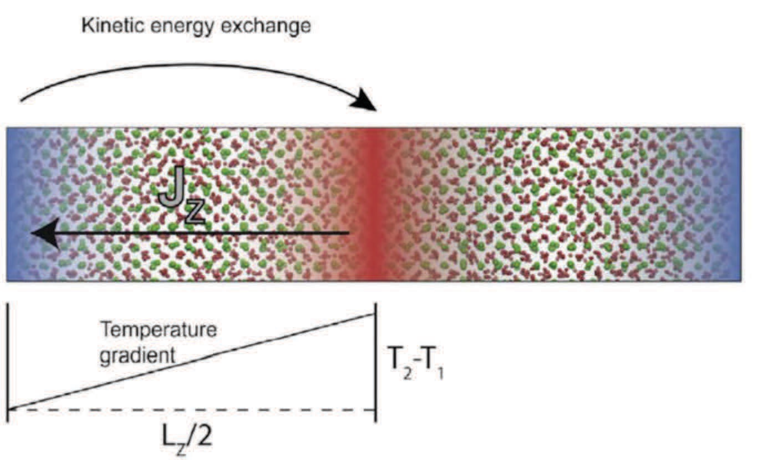
Deployment of current fuel has benefited from large experimental programs and many years of operational experience. Similar foundation less existent for advanced (ATF and non-LWR) fuel. **For *efficient* deployment of advanced fuels, it is critical that advanced modeling and simulation is** coordinated with experiment.

For pragmatic multiscale/physics-informed mod-sim – key outstanding challenge is to move beyond adding understanding to models that are sources of uncertainty, and rather quantify the uncertainty associated with engineering scale inputs derived from lower length scale models.

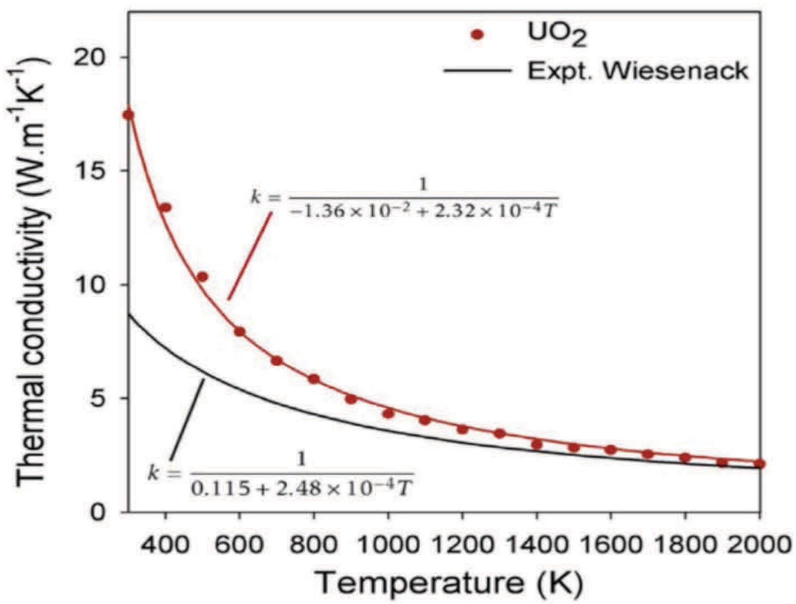
Ideally, "advanced" mod-sim should also be "flexible" mod -sim, where a similar set of tools can be used for initial "low res" scoping/reactor design, and then the same framework applied to optimization using "high res"/mechanistic adv mod sim – and integrated within innovative experimental testing program.

Do we really know everything there is to know about UO_2?

Use molecular dynamics (MD) to calculate thermal conductivity via direct method.

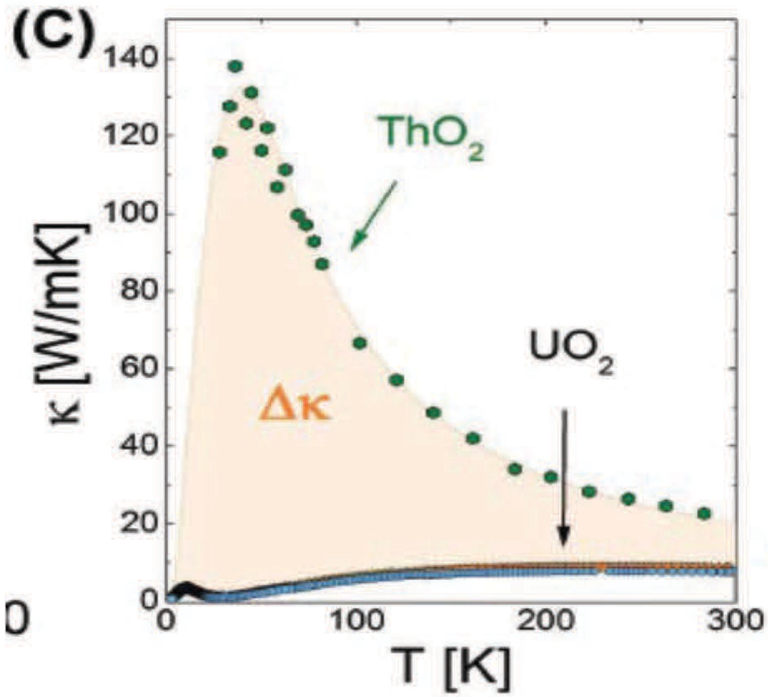


Values are significantly overestimated.



Cooper *et al. J. Nucl. Mater.* **466** 43-50 (2015)

UO_2 thermal conductivity behavior different than chemically and crystallographically similar compounds



K. Gofryk et al. *Nature Comm.* (2014)

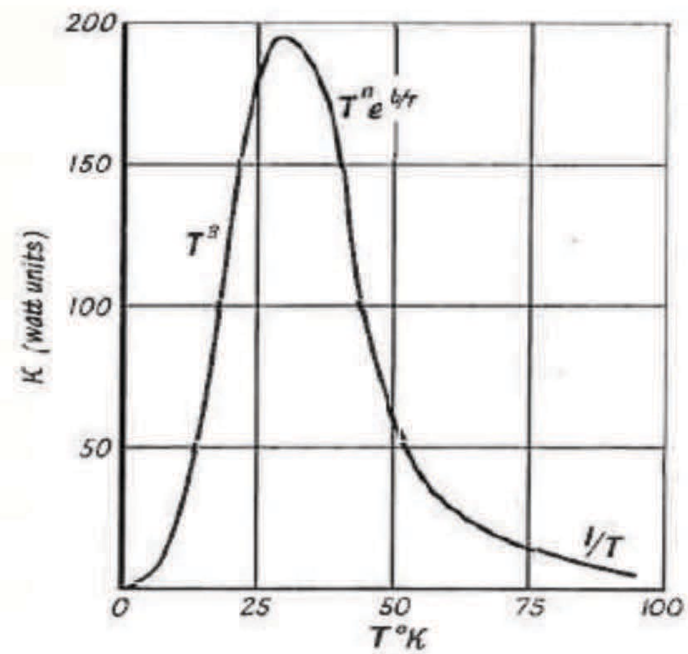


FIG. 83. Thermal conductivity of Al_2O_3 (Berman, 1958).

Phonon Scattering by Magnetic Spins

Below 30 K, UO_2 exhibits AFM ordering and above is paramagnetic. ThO_2 is diamagnetic.

In UO_2 (and not ThO_2) scattering by spin excitations on the uranium ions are responsible for the unusual shape of the thermal conductivity curve.

Scattering between phonons and spins on uranium ions occurs by phonons exciting energy levels of the magnetic ions, see e.g. Van Vleck, *Phys. Rev.* (1940), Slack & Galginaitis, *Phys. Rev.* (1964), Mattuck & Strandberg, *Phys. Rev.* (1960).

The standard Callaway model
(*Phys. Rev.* (1959))

$$\kappa = \frac{k_B}{2\pi v}\left(\frac{k_B T}{\hbar}\right)^3 \int_0^{\Theta_D/T} \frac{\tau_p x^4 e^x}{(e^x - 1)^2} dx$$

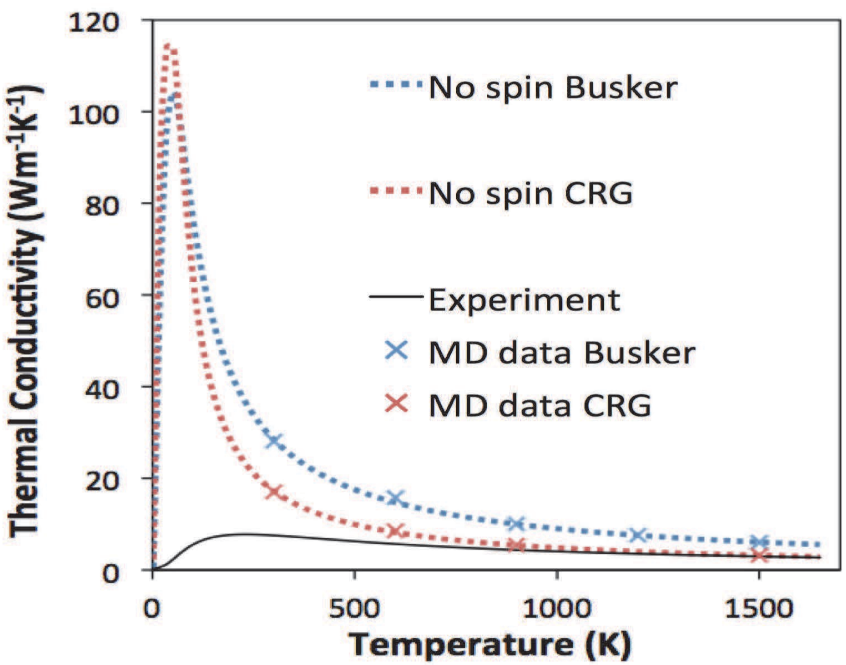
can be extended to include a spin scattering term:

$$\tau_p^{-1} = \tau_D^{-1} + \tau_B^{-1} + \tau_U^{-1} \boxed{+ \tau_S^{-1}}$$

$$\tau_S^{-1} = \sum_i \frac{C_i \omega^4}{\left(\omega^2 - \omega_{S,i}^2\right)}$$

Neelmani & Verma, Phys. Rev. B (1972).

Results without spin scattering term



$$\kappa = \frac{k_B}{2\pi v}\left(\frac{k_B T}{\hbar}\right)\int_0^{\Theta_D/T} \frac{\tau_p x^4 e^x}{(e^x-1)^2}dx$$

$$x = \hbar\omega / k_B T$$

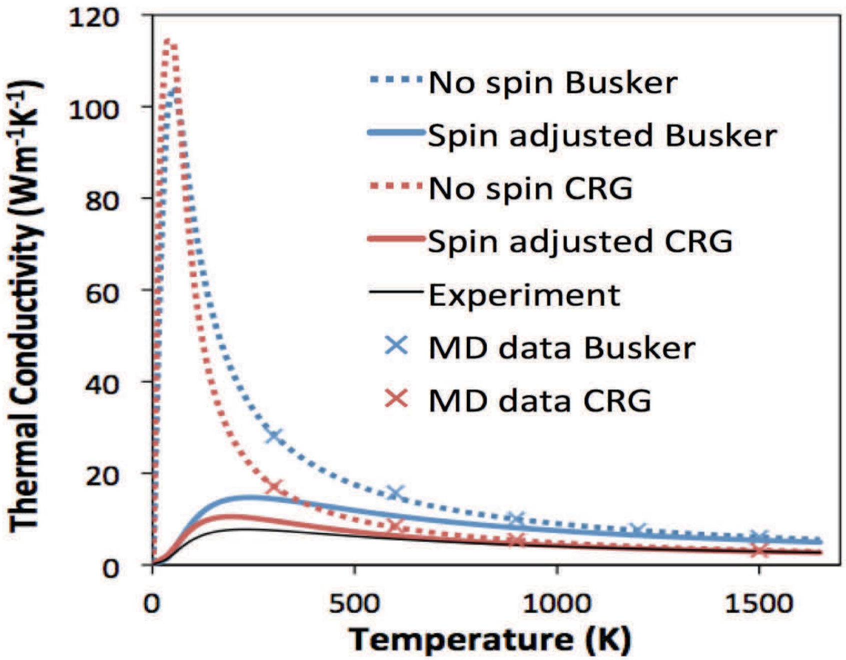
$$\tau_D^{-1} = Dx^4T^4 = D\left(\frac{\hbar\omega}{k_B}\right)^4$$

$$\tau_B^{-1} = B$$

$$\tau_U^{-1} = UT^3x^2e^{-\Theta_D/bT} = UT\left(\frac{\hbar\omega}{k_B}\right)^2 e^{-\Theta_D/bT}$$

$$\tau_S^{-1} = \sum_i \frac{C_i\omega^4}{(\omega^2-\omega_{S,i})}F_i(T)$$

Including spin scattering term



X.-Y. Liu, et al. *Physical Review Applied* **6** (2016) 044015

$$\kappa = \frac{k_B}{2\pi v}\left(\frac{k_B T}{\hbar}\right)\int_0^{\Theta_D/T} \frac{\tau_p x^4 e^x}{(e^x-1)^2}dx$$

$$x = \hbar\omega/k_B T$$

$$\tau_D^{-1} = Dx^4T^4 = D\left(\frac{\hbar\omega}{k_B}\right)^4$$

$$\tau_B^{-1} = B$$

$$\tau_U^{-1} = UT^3x^2e^{-\Theta_D/bT} = UT\left(\frac{\hbar\omega}{k_B}\right)^2 e^{-\Theta_D/bT}$$

$$\boxed{\tau_S^{-1} = \sum_i \frac{C_i\omega^4}{(\omega^2-\omega_{S,i})}F_i(T)}$$

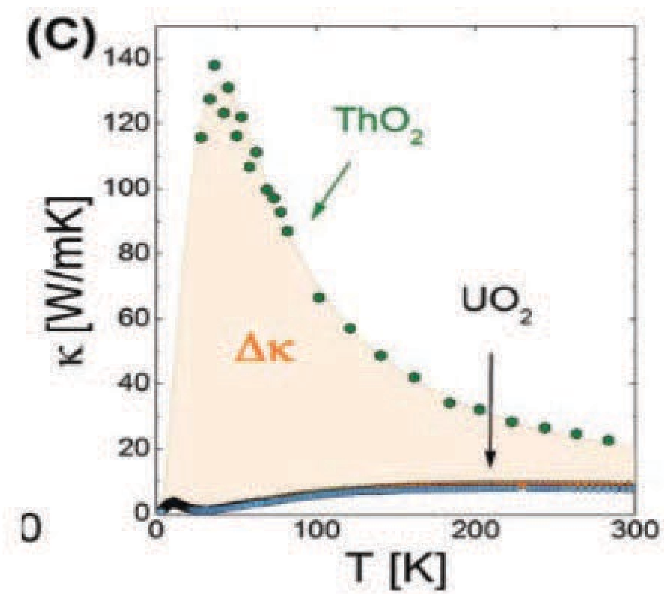
Curious anisotropic thermal conductivity in UO_2

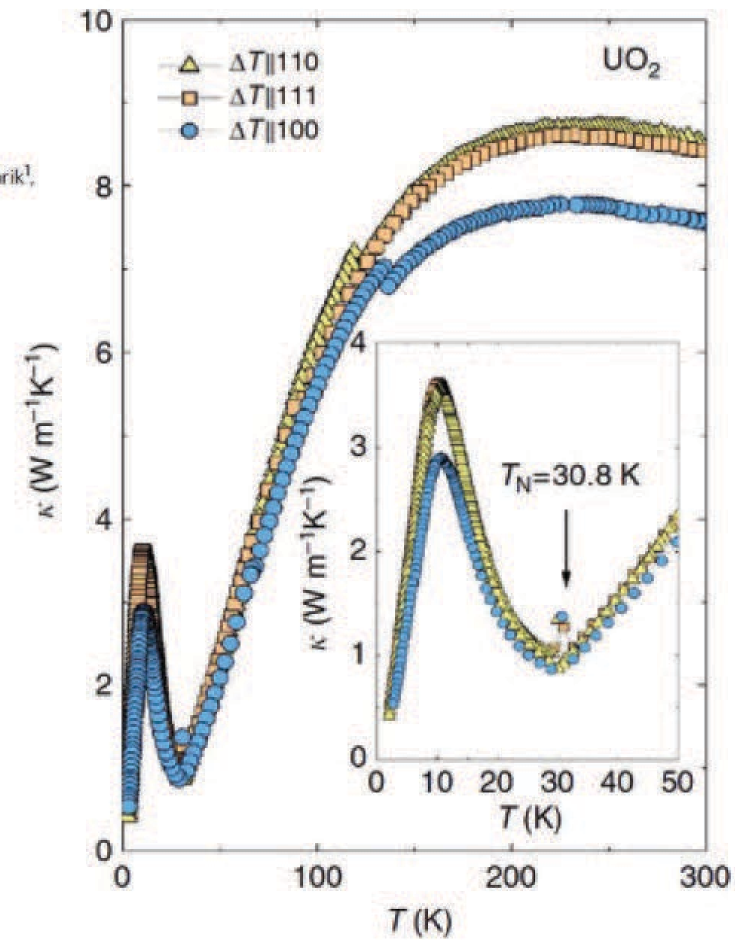
ARTICLE

Received 9 May 2014 | Accepted 27 Jun 2014 | Published 1 Aug 2014

Anisotropic thermal conductivity in uranium dioxide

K. Gofryk[1,†], S. Du[2,†], C.R. Stanek[3], J.C. Lashley[1], X.-Y. Liu[3], R.K. Schulze[1], J.L. Smith[1], D.J. Safarik[1], D.D. Byler[3], K.J. McClellan[3], B.P. Uberuaga[3], B.L. Scott[4] & D.A. Andersson[3]





Important UO_2 physics still being revealed

Recent structural analysis suggests lower symmetry structure than fluorite.

Although still cubic, perhaps a clue for thermal conductivity experiments.

Lattice and magnetic degrees of freedom in uranium dioxide are strongly coupled. Further investigation required.

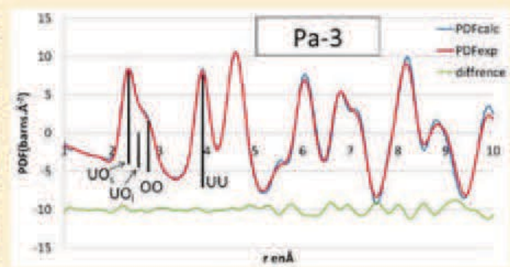
Inorganic Chemistry
Article
pubs.acs.org/IC

What Is the Actual Local Crystalline Structure of Uranium Dioxide, UO_2? A New Perspective for the Most Used Nuclear Fuel

L. Desgranges,[*,†] Y. Ma,[†] Ph. Garcia,[†] G. Baldinozzi,[‡,§] D. Siméone,[‡,§] and H. E. Fischer[∥]

[†]CEA, DEN, DEC F-13108 Saint Paul lez Durance Cedex, France
[‡]SPMS, LRC Carmen, CNRS Centrale Supélec, 92295 Châtenay-Malabry, France
[§]CEA, DEN, DMN F-91191 Gif-sur-Yvette Cedex, France
[∥]Institut Laue-Langevin, 6 rue Jules Horowitz, B.P. 156, 38042 Grenoble Cedex, France

ABSTRACT: Up to now, uranium dioxide, the most used nuclear fuel, was said to have a $Fm\bar{3}m$ crystalline structure from 30 to 3000 K, and its behavior was modeled under this assumption. However, recently X-ray diffraction experiments provided atomic pair-distribution functions of UO_2, in which UO distance was shorter than the expected value for the $Fm\bar{3}m$ space group. Here we show neutron diffraction results that confirm this shorter UO bond, and we also modeled the corresponding pair-distribution function showing that UO_2 has a local $Pa\bar{3}$ symmetry. The existence of a local lower symmetry in UO_2 could explain some unexpected properties of UO_2 that would justify UO_2 modeling to be reassessed. It also deserves more study from an academic point of view because of its good thermoelectric properties that may originate from its particular crystalline structure.



NEAMS
NUCLEAR ENERGY ADVANCED MODELING & SIMULATION PROGRAM

APPENDIX I - Fuel Qualification - NRC Perspectives

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

Fuel Qualification
NRC Perspectives

Accelerated Fuel Qualification Workshop
May 31, 2019

Topics

- Current Regulatory Approach
- Early Thoughts/Feedback on General Atomics (GA) Accelerated Fuel Qualification (AFQ) Approach
- Observations on Morning Presentations

Current Regulatory Approach

U.S.NRC
UNITED STATES NUCLEAR REGULATORY COMMISSION
Protecting People and the Environment

- All currently operating fuel designs have similar safety functions and general operating conditions
  - UO_2 pellet in zirconium-based cladding, within a fuel assembly array
  - Similar temperature, pressure, chemistry, power density, etc.
  - Fuel pellets and cladding are credited as first fission product barrier

- The staff's current regulatory approach and guidance reflect the safety functions and known failure mechanisms of Light Water Reactor (LWR) fuel
  - NRC Standard Review Plan (SRP) guidance focuses on preventing cladding failure and centerline fuel melt

Current Regulatory Approach (cont)

U.S.NRC
UNITED STATES NUCLEAR REGULATORY COMMISSION
Protecting People and the Environment

The staff's safety review provides reasonable assurance that:

1. The fuel system is not damaged as a result of normal operation and anticipated operational occurrences (AOOs),
2. The fuel system damage is never so severe as to prevent control rod insertion when it is required,
3. The number of fuel rod failures is not underestimated for postulated accidents (PAs),
4. Core coolability is always maintained.

U.S.NRC
UNITED STATES NUCLEAR REGULATORY COMMISSION
Protecting People and the Environment

Current Regulatory Approach (cont)

- Fuel-related regulations for normal operation, AOOs, and PAs:
  - 10 CFR Part 50 Appendix A, General Design Criteria (GDC):
    - GDC 10, as it relates to assuring that specified acceptable fuel design limits are not exceeded during any condition of normal operation, including the effects of AOOs.
    - GDC 27, as it relates to the reactivity control system being designed with appropriate margin and, in conjunction with the Emergency Core Cooling System (ECCS), being capable of controlling reactivity and cooling the core under post accident conditions.
    - GDC 35, as it relates to providing an ECCS to transfer heat from the reactor core following any loss of reactor coolant at a rate such that (1) fuel and clad damage that could interfere with continued effective core cooling is prevented and (2) clad metal-water reaction is limited to negligible amounts.
  - 10 CFR 50.46 as it relates to the cooling performance analysis of the ECCS using an acceptable evaluation model and establishing acceptance criteria for light-water nuclear power reactor ECCSs.

Current Regulatory Approach (cont)

- Fuel-related guidance for normal operation, AOOs, and PAs:
  - NUREG-0800 Section 4.2, “Fuel System Design”
  - NUREG/CR-6967, “Cladding Embrittlement During Postulated Loss-of-Coolant Accidents”
  - Letter from Paul M. Clifford to Timothy J. McGinty, “Technical and Regulatory Basis for the Reactivity-Initiated Accident Acceptance Criteria and Guidance, Revision 1,” March 16, 2015, ADAMS Accession No. ML14188C423

Current Regulatory Approach (cont)

- The licensing approach for LWR focuses on ensuring analysis methods and models can accurately predict and bound fuel behavior for all planned operational parameters
  - Based on empirical nature of fuel behavior models
  - Current test suite for LWR fuel based on the safety significance of the fuel, planned plant operations, and known potential failure mechanism

Current Regulatory Approach (cont)

- Fuel-related regulations for normal operation, AOOs, and PAs:
  - 10 CFR Part 50 Appendix A, General Design Criteria (GDC):
    - GDC 10, as it relates to assuring that specified acceptable fuel design limits are not exceeded during any condition of normal operation, including the effects of AOOs.
    - GDC 27, as it relates to the reactivity control system being designed with appropriate margin and, in conjunction with the Emergency Core Cooling System (ECCS), being capable of controlling reactivity and cooling the core under post accident conditions.
    - GDC 35, as it relates to providing an ECCS to transfer heat from the reactor core following any loss of reactor coolant at a rate such that (1) fuel and clad damage that could interfere with continued effective core cooling is prevented and (2) clad metal-water reaction is limited to negligible amounts.
  - 10 CFR 50.46 as it relates to the cooling performance analysis of the ECCS using an acceptable evaluation model and establishing acceptance criteria for light-water nuclear power reactor ECCSs.

Current Regulatory Approach (cont)

- Fuel-related guidance for normal operation, AOOs, and PAs:
    - NUREG-0800 Section 4.2, "Fuel System Design"
    - NUREG/CR-6967, "Cladding Embrittlement During Postulated Loss-of-Coolant Accidents"
    - Letter from Paul M. Clifford to Timothy J. McGinty, "Technical and Regulatory Basis for the Reactivity-Initiated Accident Acceptance Criteria and Guidance, Revision 1," March 16, 2015, ADAMS Accession No. ML14188C423

Current Regulatory Approach (cont)

- The licensing approach for LWR focuses on ensuring analysis methods and models can accurately predict and bound fuel behavior for all planned operational parameters
  - Based on empirical nature of fuel behavior models
  - Current test suite for LWR fuel based on the safety significance of the fuel, planned plant operations, and known potential failure mechanism

Staff Feedback on GA Approach

U.S.NRC
UNITED STATES NUCLEAR REGULATORY COMMISSION
Protecting People and the Environment

- The presentations available to the staff regarding GA's "Accelerated Fuel Qualification" approach have been high level to date. At this early stage of the process, it is unclear what would be included in a final topical report submittal, thereby limiting potential staff feedback at this time.

- The concept of reducing fuel qualification testing by leveraging greater use of computer modeling has promise, but details are needed to ensure proper guidance
  - The test matrix needs to reflect the safety significance of the fuel design, available margin, code uncertainties, or other contributing factors
  - Potential cliff-edge effects would need to be understood
  - Staff review would focus on validation requirements for predictive performance code and the applicability of historical data
  - It is currently unclear how much, if any, testing of the final fuel form is planned under the GA approach

Staff Feedback on GA Approach (cont)

U.S.NRC
UNITED STATES NUCLEAR REGULATORY COMMISSION
Protecting People and the Environment

- While the intent is a generic topical report, the information provided to date appears to be more GA-specific in nature.
  - A technology-neutral fuel qualification methodology should start at a high level to determine the safety significance and available margin of a particular fuel design and then proceed to guide the development of a design-specific fuel qualification program which incorporates an appropriate amount of testing to support model validation.

- The staff has presented a generic definition of fuel qualification at various public meetings:

  "Fuel qualification is a process which provides high confidence that physical and chemical behavior of fuel is sufficiently understood so that it can be adequately modeled for both normal and accident conditions, reflecting the role of the fuel design in the overall safety of the facility. Uncertainties are defined so that calculated fission product releases include the appropriate margins to ensure conservative calculation of radiological dose consequences."

May 31, 2019 9

U.S.NRC
UNITED STATES NUCLEAR REGULATORY COMMISSION
Protecting People and the Environment

Staff Feedback on GA Approach (cont)

- Licensing requirements will depend on desired license type
    - Prototype plant licenses allow for construction and operation to increase the database, but could include operational restrictions, additional safety requirements, site location restrictions, or testing requirements.
    - Additional guidance regarding prototype and test reactor licensing can be found in “A Regulatory Review Roadmap For Non-Light Water Reactors”, ADAMS Accession Number (ML17312B567).

- Early and frequent engagement with the staff is highly recommended

Observations on Morning Presentations

GENERAL ATOMICS
P.O. BOX 85608 SAN DIEGO, CA 92186-5608 (858) 455-3000