PRIFYSGOL
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Dr. Simon Middleburgh FIMMM
Reader in Nuclear Materials

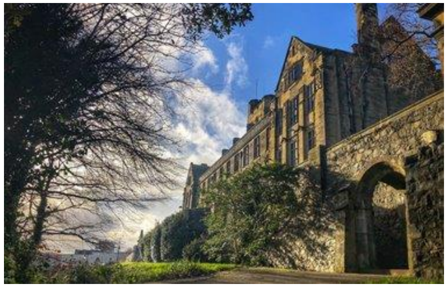
NUCLEAR**FUTURES**
Bangor

Mechanistic modelling of nuclear fuels for rapid commercial deployment

Modelling in Nuclear Science and Engineering
5th November 2020

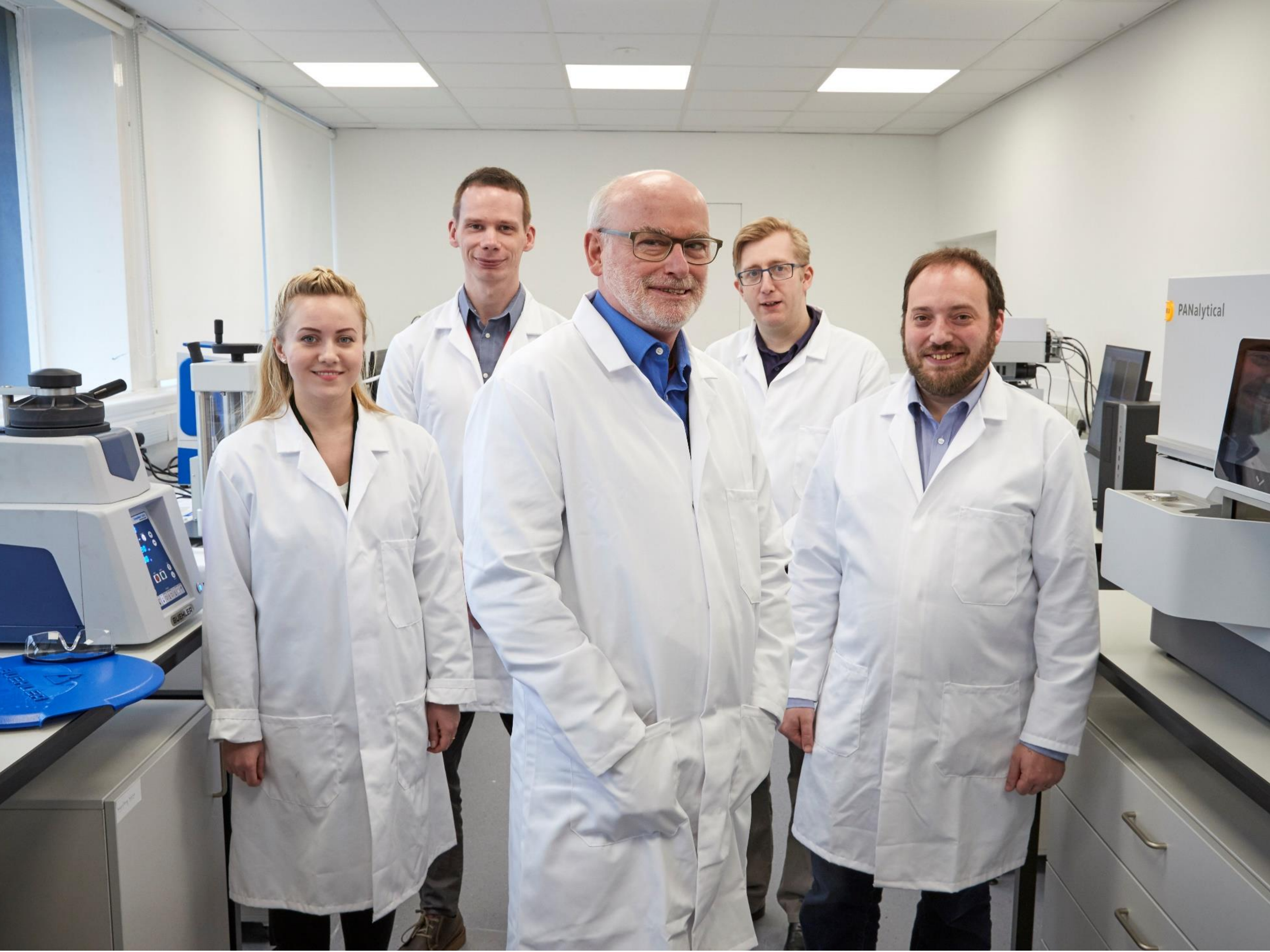
Who am I?

- Grew up in Worcestershire.
- Finished my Ph.D. in 2012 at Imperial College London
  - Sponsored by Westinghouse Electric Company.
  - Worked on modelling of doped fuels, burnable absorbers and beryllium.
- Moved to Australia to work at ANSTO (modelling and experiment).
- Took up a senior engineer role at Westinghouse Electric Sweden working on new fuel and fuel performance codes.
- Joined Bangor University in 2018.
- Published ~70 papers and 13 patents.
- Currently supervise 6 industry sponsored PhD students.



People

- **Bill Lee FREng:** Nuclear Materials: Fuels and Wastes, Ceramics.
- **Laurence Williams OBE FREng:** Nuclear Policy, Safety, Security, Radioactive Waste and Regulation.
- **Simon Middleburgh:** Nuclear fuel materials manufacture, characterisation and modelling (DFT).
- **Marcus Dahlfors: T**hermal hydraulics and reactor physics.
- **Michael Rushton:** Materials characterisation and modelling.
- **PDRAs (Iuliia Ipatova** – experimental. **Lee Evitts -** modelling, **Phylis Makurunje** – experimental).
- Visiting Profs and Industry Associates: **John Idris Jones** (Snowdonia Enterprise Board), **Linda Warren** (Environmental Law), **Antoine Claisse** and **Mattias Puide** from Westinghouse, **John Lillington** from Jacobs and **Matthew Gilbert** (AWE).


PANalytical
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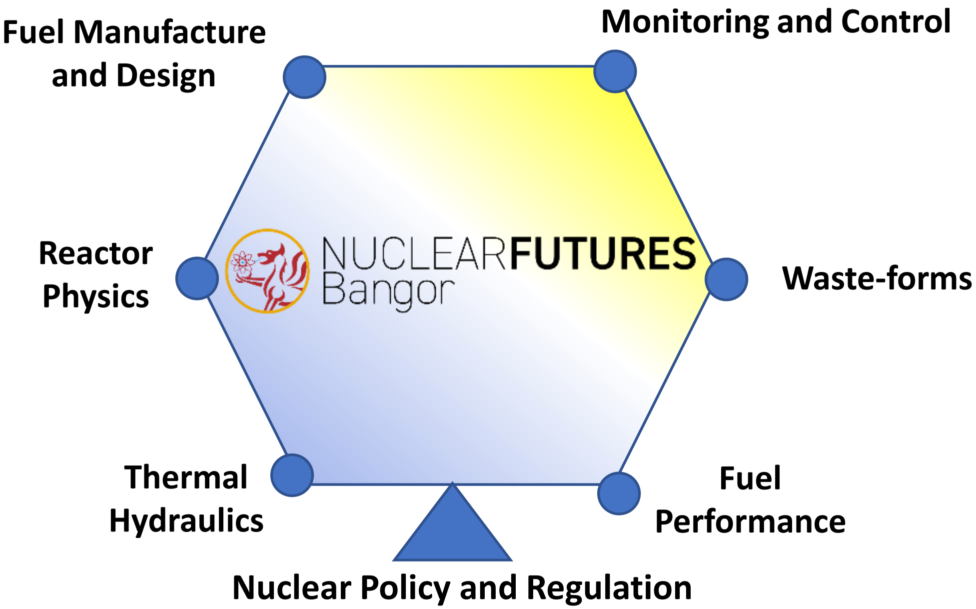
Llywodraeth Cymru
Welsh Government
Cronfa Datblygu Rhanbarthol Ewrop
European Regional Development Fund

Initial Focus Areas



Partnering for Performance
Partnering for Prosperity
Partnering for Change

Built for Collaboration

SUPERCOMPUTING WALES
UWCHGYFRIFIADURA CYMRU

The Open University

Llywodraeth Cymru
Welsh Government

Westinghouse

Lancaster University

wood.

NUCLEAR AMRC

AWE

NATIONAL NUCLEAR LABORATORY

EPRI

LeadCold

The University Of Sheffield.

HITACHI
Inspire the Next

TWI

University of BRISTOL

Australian Government

ANSTO

Imperial College London

tokamak energy

DE LA RECHERCHE À L'INDUSTRIE
cea

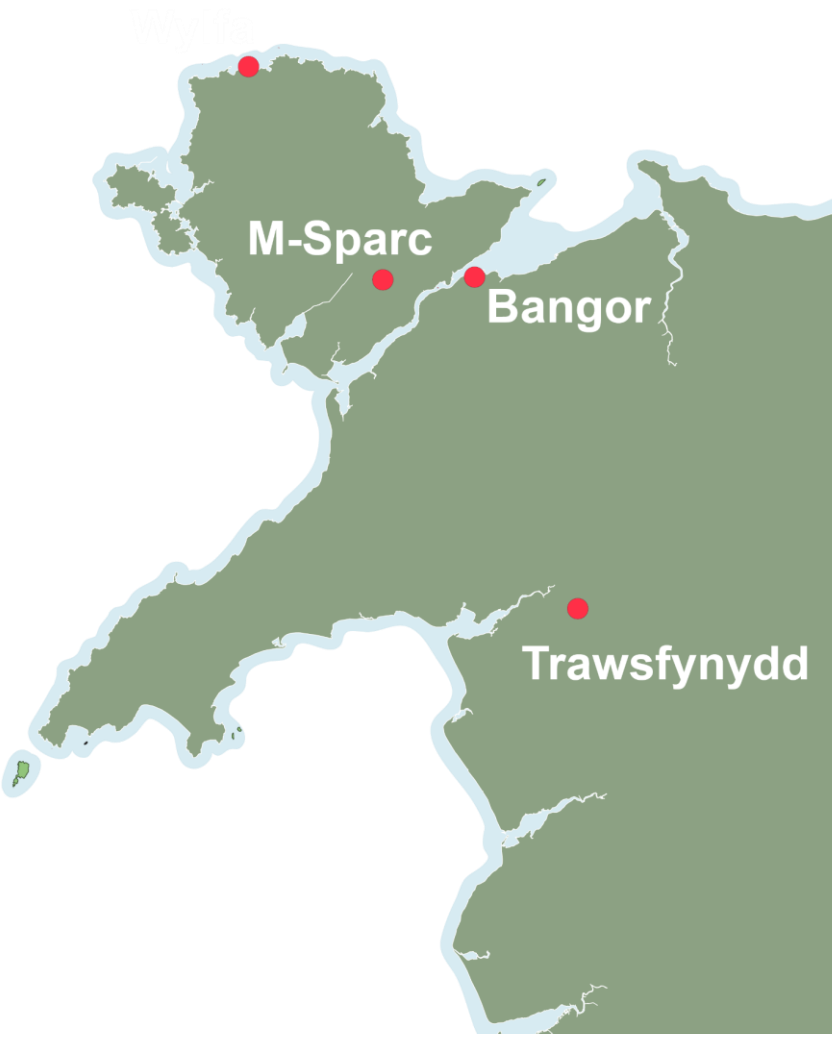
HORIZON
NUCLEAR POWER

Los Alamos
NATIONAL LABORATORY
EST. 1943

Canadian Nuclear Laboratories

MANCHESTER
1824
The University of Manchester

Vision for N Wales Low C Energy Triangle



- Bangor – University, Coleg Menai with apprentice, UG and PG training and links to local industry and community.

- Anglesey – Reactor at Wylfa, Thermal Hydraulics facility and Low C Energy Centre of Excellence at M-SParc including central research labs and facilities and innovation hub.

- Trawsfynydd – Small Modular Reactor/Advanced Modular Reactor and satellite Low C Energy Centre of Excellence linked to reactor type and regional hydro electric power and water storage capability.

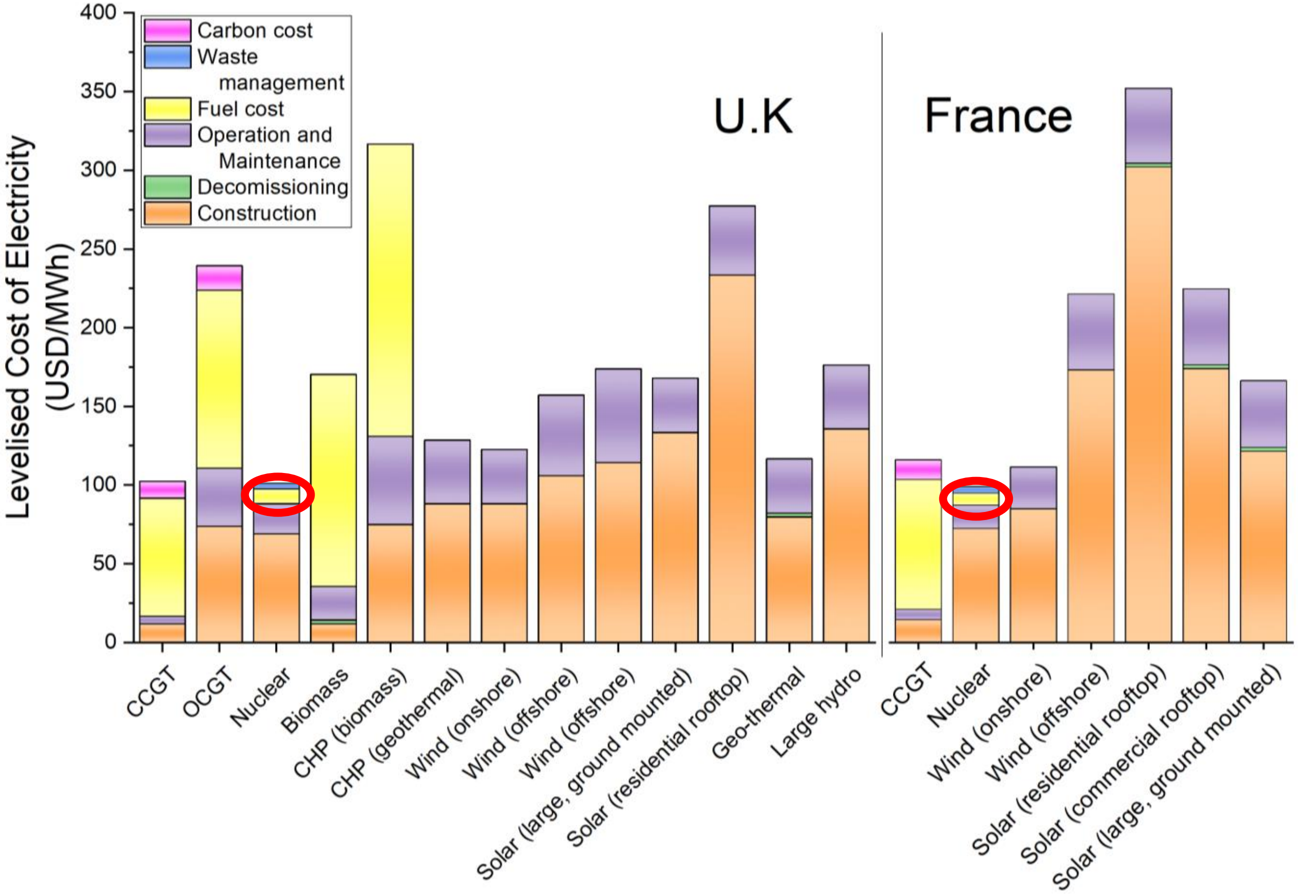
Accident Tolerant Fuels: A big deal

- First time the industry has pushed to make big changes in its fuel materials since the early 1960s.
- Bring a new generation of scientists and engineers into the industry with a deep understanding of fuel.
- Support a major UK business growth area.

However… the focus on accidents has not been *great* in the eyes of the public and economically some of these concepts do not make sense.

The future of ATF

Improving the economics of nuclear fuel



Fuel is cheap… at least right now.

So how does one impact the cost?

Improving economics with fuel

Fuel costs are low so economic advantage must be attained from elsewhere.

Within the **operation and maintenance** costs, planned and unplanned outages represent the largest impact on plant capacity factor.

- Planned outages can be reduced by increasing the cycle lengths.
- Un-planned outages can be reduced by increasing the reliability of fuel.

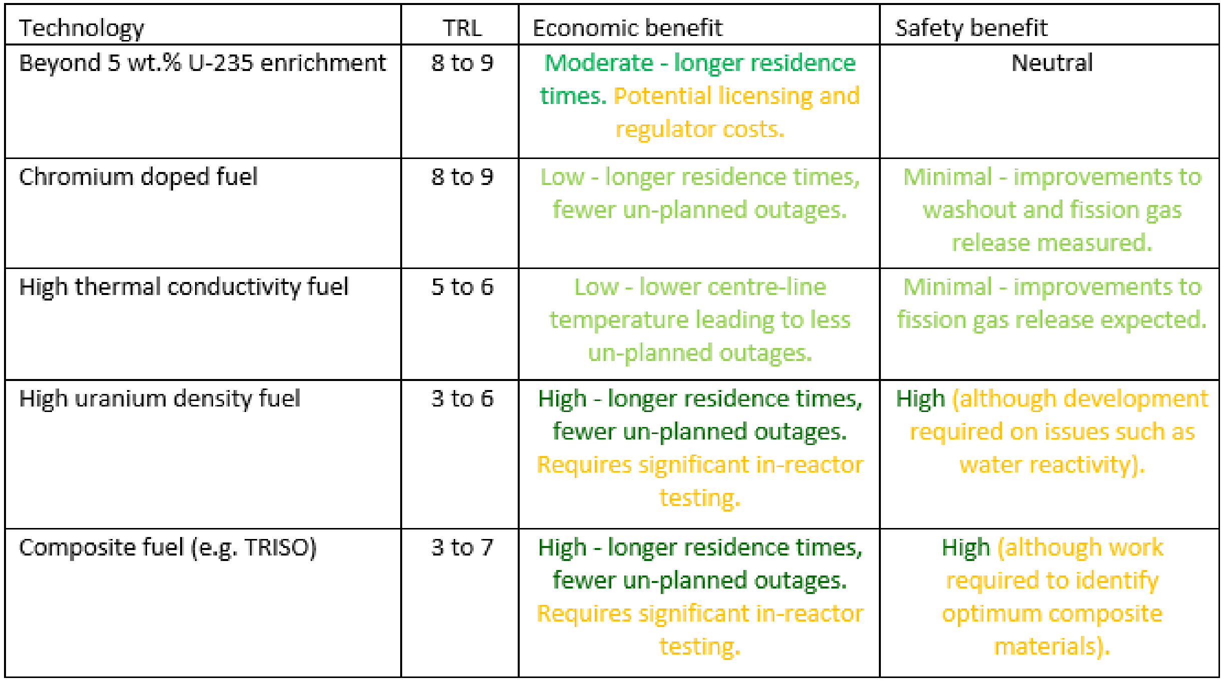
Planned outages can be reduced by utilising longer fuel cycles

Major ATF benefits come from advanced pellet materials that incorporate higher densities of ^{235}U.

- UN
- UC
- UB_2
- U_3Si_2
- High density UO_2
- Composites of the above

New production facilities required…

Table 1 - Assessment of current accident tolerant fuel pellet technologies with respect to their technological readiness level (TRL), estimated economic benefit and estimated safety benefit.



Technology	TRL	Economic benefit	Safety benefit
Beyond 5 wt.% U-235 enrichment	8 to 9	Moderate - longer residence times. Potential licensing and regulator costs.	Neutral
Chromium doped fuel	8 to 9	Low - longer residence times, fewer un-planned outages.	Minimal - improvements to washout and fission gas release measured.
High thermal conductivity fuel	5 to 6	Low - lower centre-line temperature leading to less un-planned outages.	Minimal - improvements to fission gas release expected.
High uranium density fuel	3 to 6	High - longer residence times, fewer un-planned outages. Requires significant in-reactor testing.	High (although development required on issues such as water reactivity).
Composite fuel (e.g. TRISO)	3 to 7	High - longer residence times, fewer un-planned outages. Requires significant in-reactor testing.	High (although work required to identify optimum composite materials).

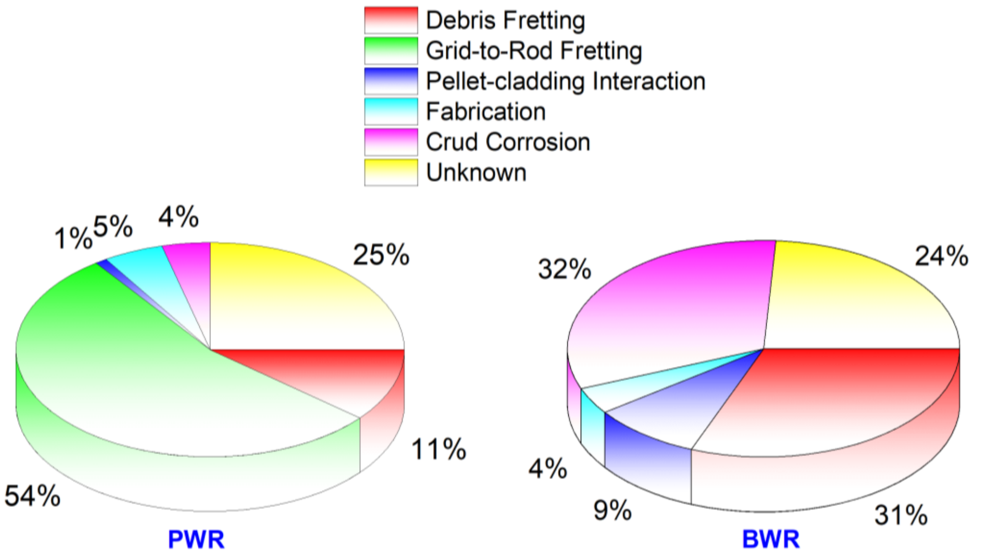
Current commercial fuels are mostly limited to 5wt.% ^{235}U enrichment. All concepts, including standard UO_2 can gain benefit for >5wt.% ^{235}U.

Unplanned outages can be reduced by increasing fuel reliability

Major ATF benefits come from advanced cladding materials.

Hard coatings that provide resistance to fretting and provide improvements related to corrosion (*incidentally* helping in severe accidents). Provide the most benefit.

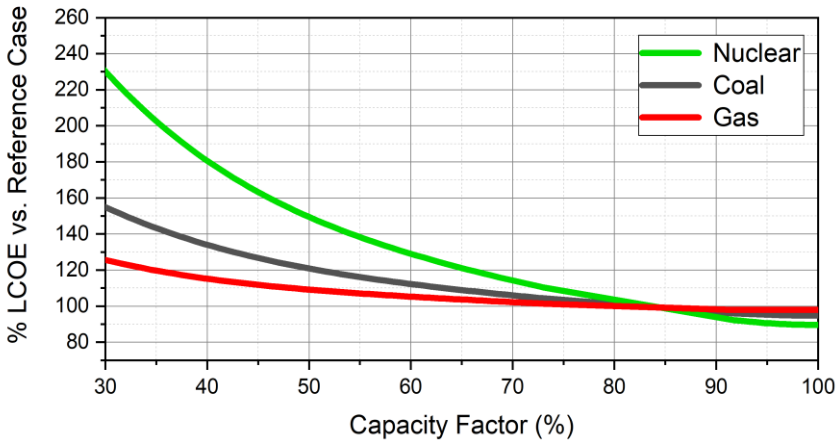
Clear leader here is the potential coated Zr-cladding concepts. Cr-coatings for PWRs.

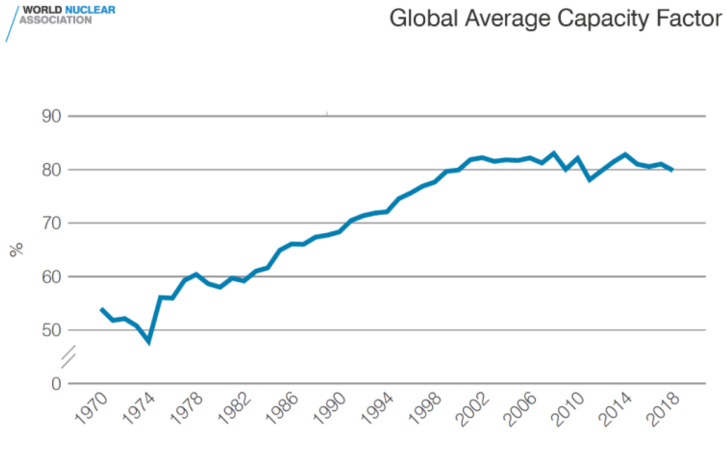


IAEA Nuclear Energy Series NF-T-2.1 "Review of Fuel Failures in Water Cooled Reactors" Chapter 3, (2010).

Maintaining high capacity factor key!

- Nuclear really suffers when it is not being used at full capacity according to economical assessment.
- New fuel concepts must equal or better reliability and performance compared to current generation of fuel.
- Capacity factor must be reliably increased across the fleet of nuclear generating stations for economic benefits.
- 5-10% reduction in cost achievable by increasing capacity factor from 80% to 90%. Dwarfs long-term capital costs for many ATF concepts (not all).
- Load follow not sensible – but diversifying production is. **Co-generation** the key to deep decarbonization.





Source: World Nuclear Association, IAEA PRIS

www.neimagazine.com

September 2020

NUCLEAR ENGINEERING INTERNATIONAL

Opinion
Jeremy Gordon discusses the recent disaster in Beirut

Operation
WNA looks at the benefits of long-term operation

Fuel & fuel cycle
Flash sintering for nuclear fuel manufacturing

Fuel & fuel cycle
Upgrading Hunterston B during a pandemic

Fuel data
Technical data for a range of nuclear fuel designs

Fuelling Net Zero
The UK's Advanced Fuel Cycle Programme

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serving the nuclear industry since 1956

Simon Middleburgh

Ser Cymru Reader in nuclear materials at the Nuclear Futures Institute at Bangor University

Mustafa Bolukbasi

First-year Ph.D. student in Nuclear Futures Institute at Bangor University

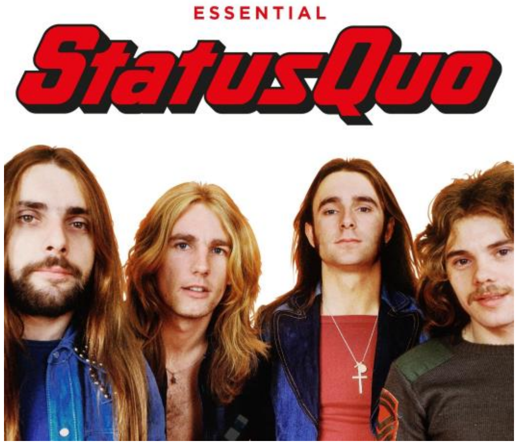
Dave Goddard

Laboratory fellow, nuclear fuel manufacturing at National Nuclear Laboratory

Enhancing economics with ATF

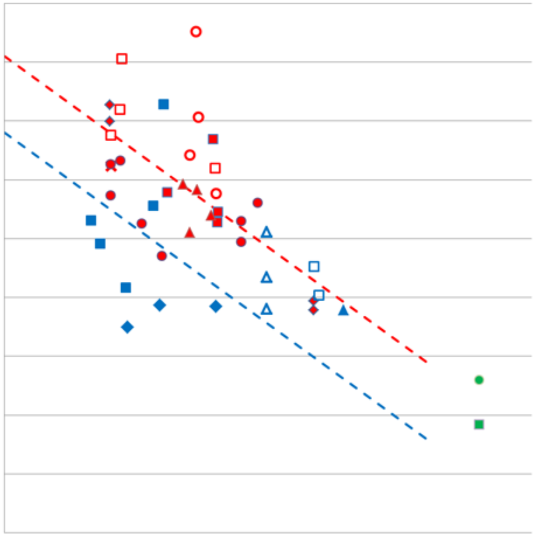
Adoption of advanced technology fuels (ATF) is on the rise, but their economic impact is poorly understood. The UK's Advanced Fuel Cycle Programme is shifting understanding. By **Simon Middleburgh, Mustafa Bolukbasi** and **Dave Goddard**

Past



- Lots of in-reactor testing producing lots of empirical data.
- Expensive (a typical reactor experiment with PIE costs ~£1M per rod).
- Decades to make very minor changes to fuel.
- Supported the status-quo.
- Stunted progress in the nuclear energy industry.

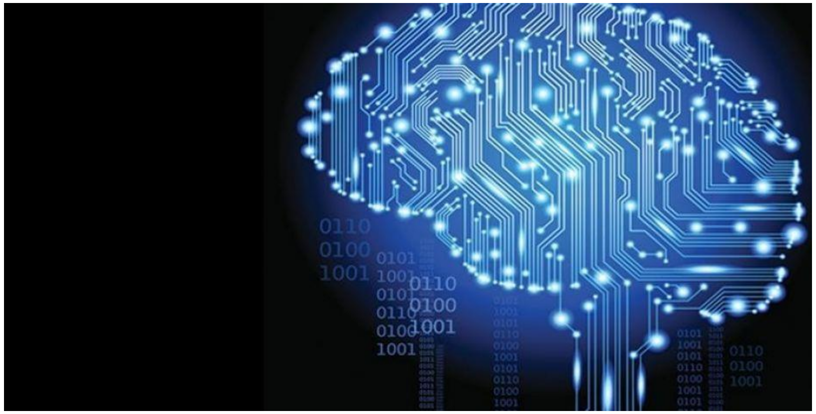
Sexy hardware



Operational experience making up for dubious statistics

Future

- Mechanistic understanding of fuel behaviour.
- Models that allow one to reliably extrapolate between measured points.
- Reduces burden on test reactor facilities.
- Reduces times to assure regulator.
- Reduces cost.

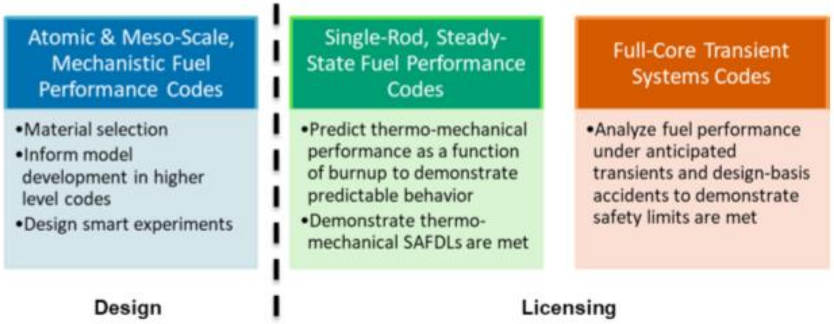


Sexy hardware

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

PROJECT PLAN TO PREPARE THE U.S. NUCLEAR REGULATORY COMMISSION FOR EFFICIENT AND EFFECTIVE LICENSING OF ACCIDENT TOLERANT FUELS

Version 1.0



Atomic & Meso-Scale, Mechanistic Fuel Performance Codes

- Material selection
- Inform model development in higher level codes
- Design smart experiments

Single-Rod, Steady-State Fuel Performance Codes

- Predict thermo-mechanical performance as a function of burnup to demonstrate predictable behavior
- Demonstrate thermo-mechanical SAFDLs are met

Full-Core Transient Systems Codes

- Analyze fuel performance under anticipated transients and design-basis accidents to demonstrate safety limits are met

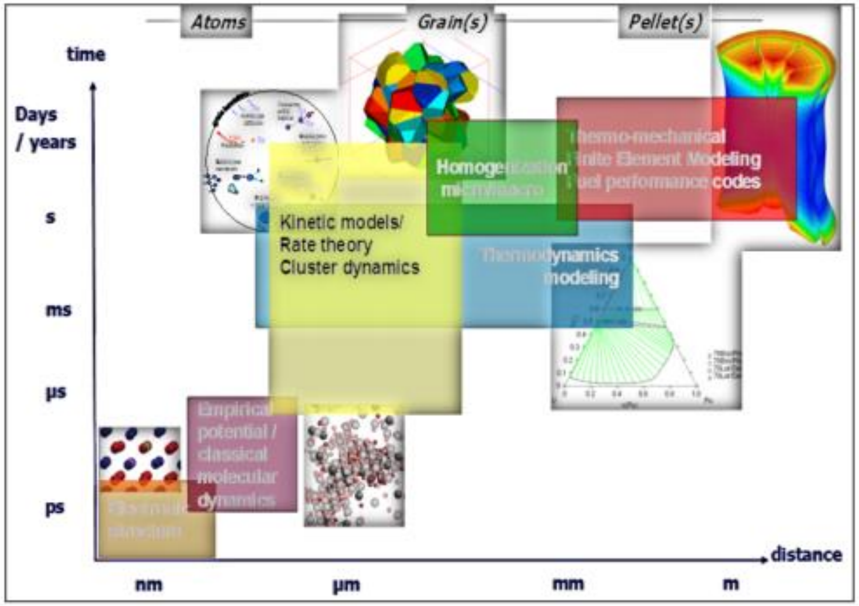
Design

Licensing

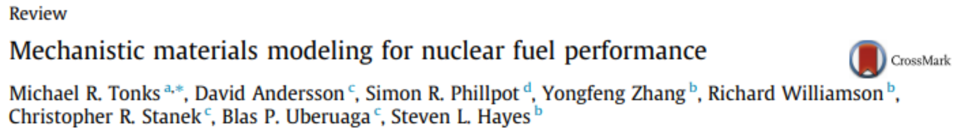
Figure 6.1 Example applications and use of code families in the area of fuel performance

SAFDL = Specified Acceptable Fuel Design Limit

Licensing and fuel performance



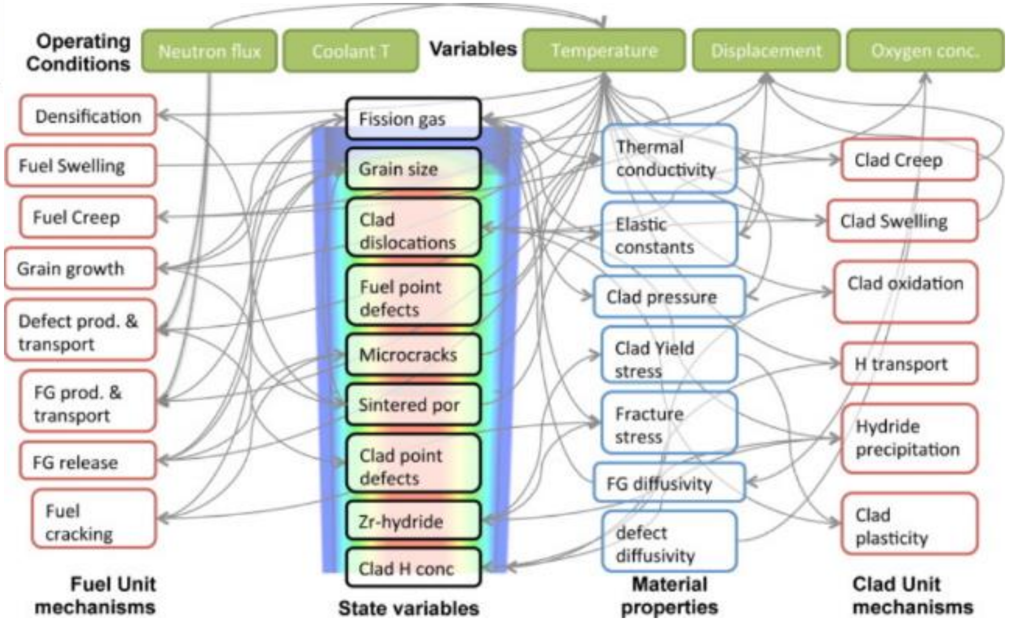
Combine multi-scale modelling with existing fuel performance code architectures to enable rapid and evolving mechanistic improvements.

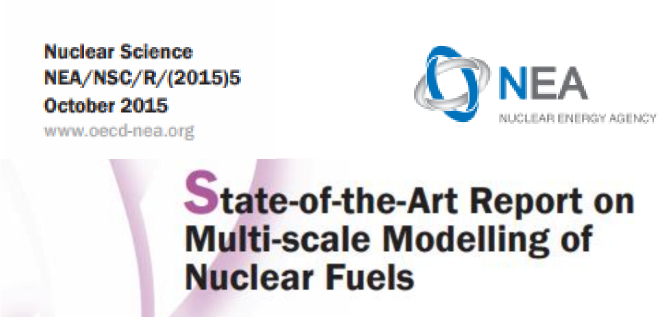


Review

Mechanistic materials modeling for nuclear fuel performance

Michael R. Tonks [a,*], David Andersson [c], Simon R. Phillpot [d], Yongfeng Zhang [b], Richard Williamson [b], Christopher R. Stanek [c], Blas P. Uberuaga [c], Steven L. Hayes [b]





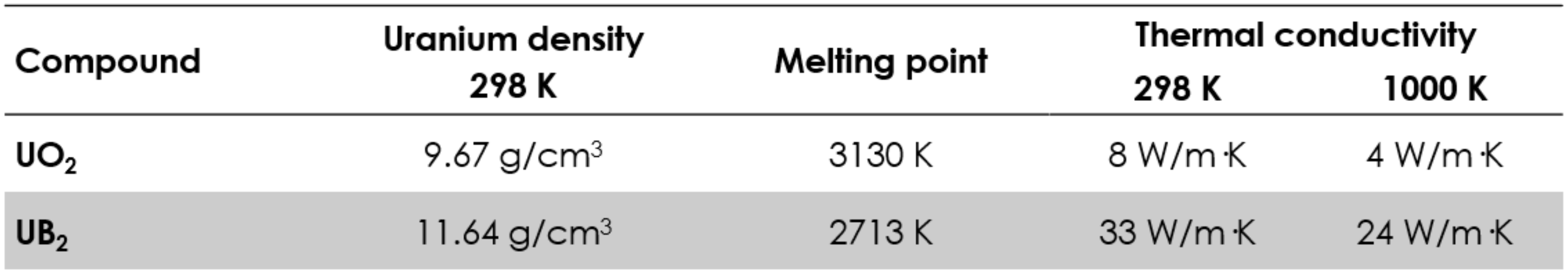
Nuclear Science
NEA/NSC/R/(2015)5
October 2015
www.oecd-nea.org

NEA
NUCLEAR ENERGY AGENCY

State-of-the-Art Report on Multi-scale Modelling of Nuclear Fuels

A new fuel - UB_2

Collaborating with Westinghouse (Mattias Puide), NNL (Dave Goddard & Emma Vernon) and University of Manchester (Joel Turner) – Project leads: **Fabio Martini and Lee Evitts at Bangor**



Compound	Uranium density 298 K	Melting point	Thermal conductivity	
			298 K	1000 K
UO_2	9.67 g/cm^3	3130 K	8 W/m·K	4 W/m·K
UB_2	11.64 g/cm^3	2713 K	33 W/m·K	24 W/m·K

- Why UB_2?
  - Can be used as a fuel or a neutron absorbing material
  - Higher density of U than UO_2 so can use more robust packaging
  - Ultra-high temperature ceramic
- Issues?
  - No commercial synthesis route)
  - Unknown reaction with water
  - Unknown properties

Materials synthesis with the help of atomic scale modelling

Synthesis of candidate advanced technology fuel: Uranium diboride (UB_2) via carbo/borothermic reduction of UO_2

J. Turner [a, *], F. Martini [b], J. Buckley [a], G. Phillips [a], S.C. Middleburgh [b], T.J. Abram [a]

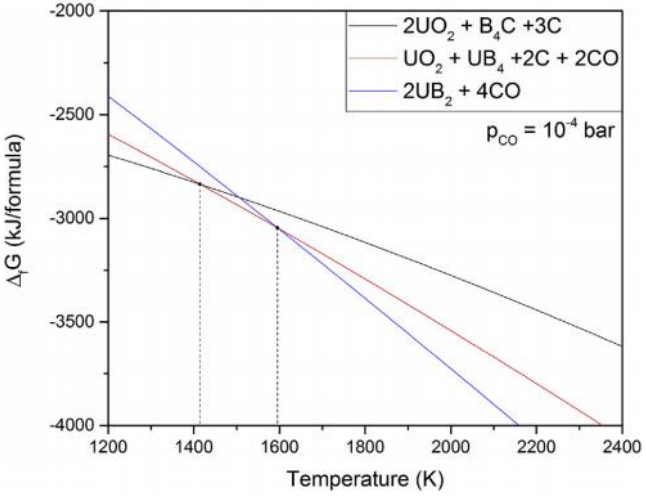


Fig. 1. Free energy of formation of the three reactions considered in Table 3, calculated at a CO pressure of 10^{-4} bar.

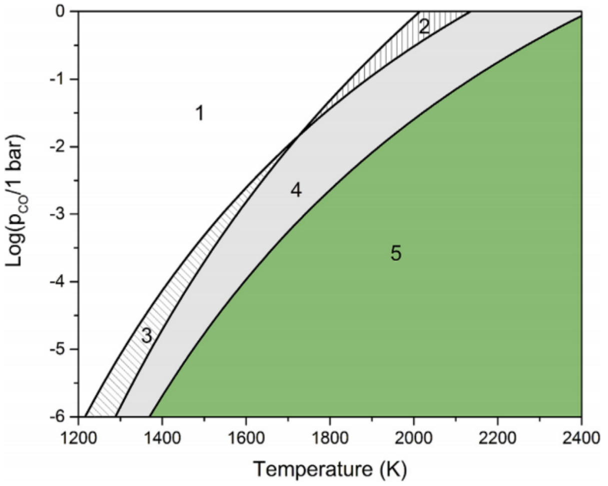
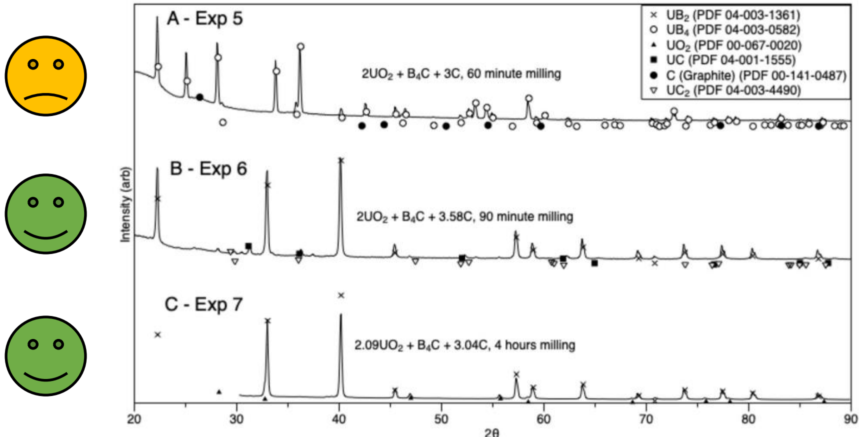


Fig. 2. Phase diagram for the condensed phases of the reaction mixture for the borocarbothermal synthesis of UB_2. Region 1: UO_2, B_4C and C; Region 2: UO_2, UB_4, B_2O_3 and C; Region 3: UO_2, UB_4 and C; Region 4: UO_2, UB_4, C and B_2O_3 may form as an intermediate product; Region 5: UB_2.



We can make it!

(We all had issues with U_3Si_2…)

Materials property discovery to accelerate licensing with the help of atomic scale modelling (density functional theory)

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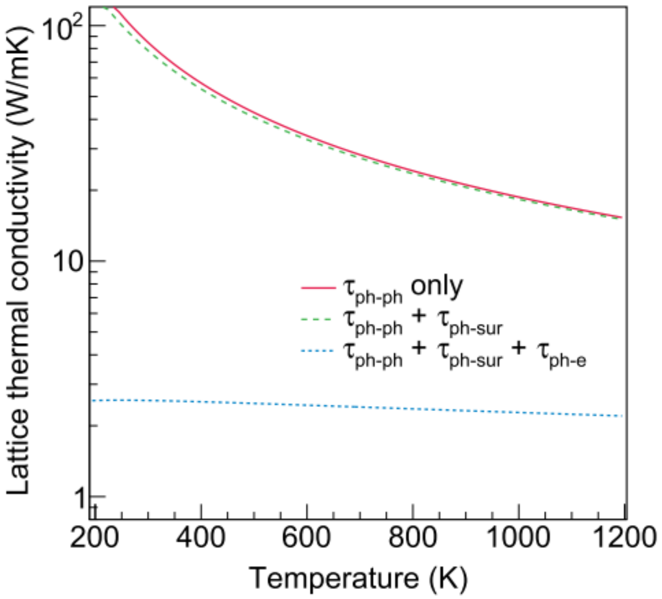
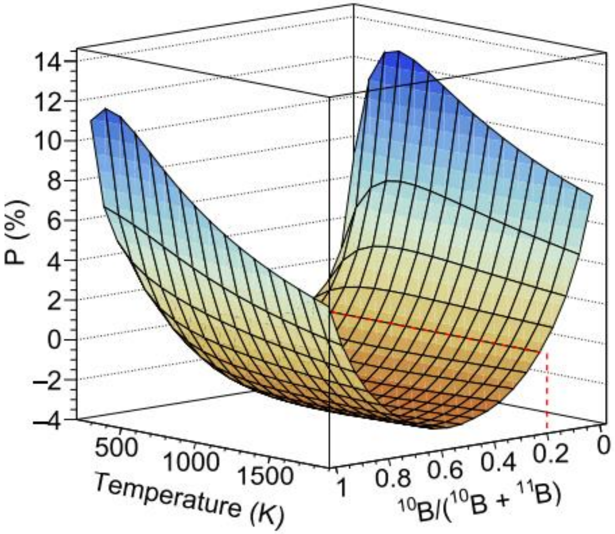
Influence of boron isotope ratio on the thermal conductivity of uranium diboride (UB_2) and zirconium diboride (ZrB_2)

L.J. Evitts [a,*], S.C. Middleburgh [a], E. Kardoulaki [b], I. Ipatova [a], M.J.D. Rushton [a], W.E. Lee [a,c]



Thermal conductivity of UB_2 significantly affected by phonon-electron scattering.



B isotope ratio has a measurable impact on thermal conductivity in ZrB_2 but not UB_2

Significant work to be done predicting the electron conductance impact on T_C

Thermophysical and mechanical property assessment of UB_2 and UB_4 sintered via spark plasma sintering

E. Kardoulaki [a,*], J.T. White [a], D.D. Byler [a], D.M. Frazer [a], A.P. Shivprasad [a], T.A. Saleh [a], B. Gong [b], T. Yao [b,c], J. Lian [b], K.J. McClellan [a]

Reducing operational margins of existing fuel with improved, mechanistic understanding (molecular dynamics)

Australian Government

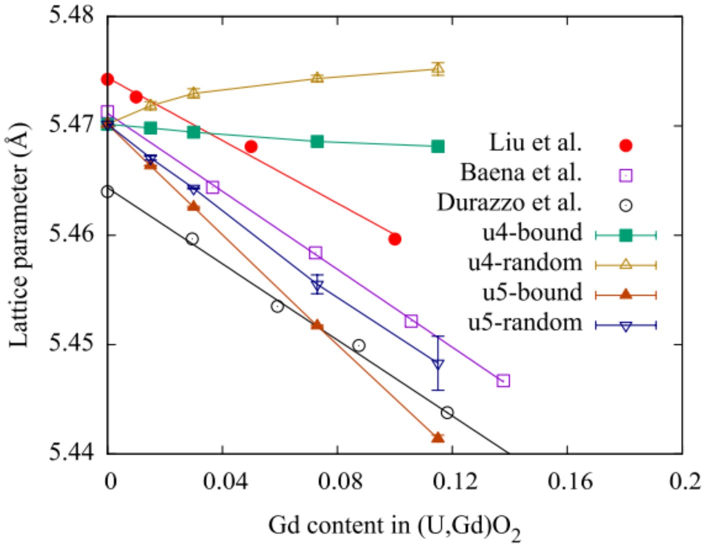
ANSTO

Imperial College London

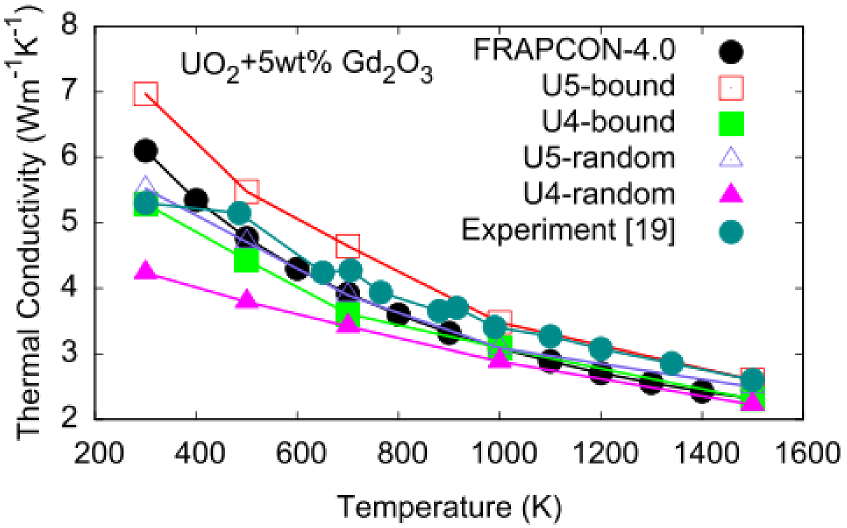
Los Alamos NATIONAL LABORATORY EST.1943

Thermal conductivity variation in uranium dioxide with gadolinia additions

M.J. Qin [a, *], S.C. Middleburgh [b, c], M.W.D. Cooper [d], M.J.D. Rushton [c, e], M. Puide [b], E.Y. Kuo [a], R.W. Grimes [e], G.R. Lumpkin [a]



Lattice parameter variation suggests that Gd is accommodated by U^{5+} ions in commercial fuel (dark blue data).



Thermal conductivity of material changes depending on Gd_2O_3 accommodation mechanism.

Changes in chemistry within the fuel during operation could alter the accommodation mechanism, changing the thermal behaviour.

Once integrated into a mechanistic fuel performance code, impacts could be investigated.

Summary

- Need for new fuels growing due to need to improve economics, fuel new reactors and increase sustainability.
- Licensing new fuels can be accelerated by using modelling methods including atomic scale modelling.
- Combine mechanistic models with experimental data to improve predictability.
- New fuels such as UB_2 and composite fuels could be first to be licensed in such a manner.
- Existing fuel operation margins can be reduced with better understanding.

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Diolch!
Thank you!

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