

Materials Modelling and Simulation for Nuclear Fuels (MMSNF) Workshop

David Braley Health Sciences Centre, Room 6001
1280 Main St. West, Hamilton, ON
Nov. 28-30, 2023

“Modelling approaches to best align with experimental programmes to enhance understanding of modern fuels and accelerate the design and qualification cycle of advanced reactor fuel materials.”

Programme

Talks are delivered by the first author unless indicated by an underline.

Tuesday November 28, 2023

- 9:00 **Tour of McMaster facilities**
Pickup: Sheraton Hamilton Hotel, 116 King Street West, Hamilton, ON
- 12:00 **Registration**
12:00 *Lunch – Sandwiches and refreshments*
12:30 **Welcome and announcements.**
Organizing committee, J. Preston (MU), D. Radford (CNL), M. Freyss (CEA)
- 13:10 **Invited talk: Should AI Go Nuclear?**
M. Stan (A1A)

Session A: Electronic Structure / Atomistic

Chair: D. Radford

- 13:30 **Bridging Length and Time Scales: Computational Modelling of Zirconium-based Alloys**
L Béland (QU), Y Luo (QU), A Ghorbani (QU), A Kamath (QU), C Dai (CNL, QU), P Saidi (CNL, QU), M Mohsini (QU), C Varvenne (CINaM), M Daymond (QU)
- 13:50 **Diffusional creep in UO₂ predicted by atomistic and meso-scale simulations**
C. Galvin, W. Neilson, T Matthews, D Andersson, M Cooper (LANL)
- 14:10 **Development of machine learning interatomic potential for molten NaCl, liquid sodium, and chlorine gas**
H Sun (QU), M Christopher (CNL), T Edmanuel (CNL) and L Béland (QU)
- 14:30 *Coffee break*
- 14:50 **Volatile fission products behaviour in oxide fuels: First principles calculation contribution to multiscale modeling of stress corrosion cracking**
M Gascoir (CEA) V Klosek (CEA), M Freyss (CEA), I C Njifon (CNL)
- 15:10 **Accident Tolerant Fuel for Generation IV and Small Modular Reactors; Simulation and Experiments**
J. Szpunar, J. Ranasinghe (USK)
- 15:30 **Panel discussion**

Reception and poster session

- 16:00 *Flash talks*
16:30 *Poster session (listed below)*

Wednesday November 29th

- 8:30 *Arrival refreshments*
8:30 **Announcements**

Session B: Mesoscale

Chair: N. Ofori-Opoku

- 8:40 **Influence of irradiation induced defects on thermal conductivity of oxide fuels**
M Khafizov (OSU), A Khanolkar (INL), K Bawane (INL), M Jin (Penn State U), J Ferrigno (OSU), S Adnan (OSU), E Nosal (OSU), L Malakkal (INL), B Kombiah (INL), A el Azab (PU), Y Zhang (UWM), L He (NCSU), D Hurley (INL)
- 9:00 **Mesoscale modeling and experimentation of zirconium alloys**
Hamid Abdolvand (UWO)
- 9:20 **Direct validation of numerical twins of nuclear fuel microstructures using micro-tomography**
L Moutin (CEA), J Meynard (CEA), F Adenot (CEA), Vincent Bouineau (CEA), C Duguay (CEA), L Fayette (CEA), M Josien (CEA), A King (PB), M Bornert (UGE), R Masson (CEA)
- 9:40 **Multi-scale simulation of Fuel-Cladding Chemical Interaction in U-Zr Metallic Fuel**
L K. Aagesen, J Hirschhorn, C Jiang (INL)
- 10:00 *Coffee break*
- 10:20 **Modeling the impact of coatings on fuel loss with cermet fuels for nuclear thermal propulsion**
V Yadav (UF), M. R. Tonks (UF), J Rosales (NASA)
- 10:40 **Phase-field modeling of incipient melting in oxidized fuel: a new step toward multicomponent systems**
C. Introini, R. Le Tellier (CEA)
- 11:00 **Phase-field approach to diffusion-driven fracture**
B. Bourdin (MU)
- 11:20 *Discussion*
- 12:00 *Lunch*
- 12:30 **OPG Electrifying Life: Nuclear Refurbishments and New Builds**
A Aamir (OPG)

Session C: Thermodynamics

Chair: T M Besmann

- 13:30 **Coupled modelling of thermodynamic and physicochemical properties of NaF-KF-UF₄ fuel molten salt**
L Ruszczynski (DU, ST), J Rothe (KIT), K Dardenne (KIT), Anna L. Smith (DU)

- 13:50 **Thermochemical Modeling of Complex Composition Molten Salt Reactor Fuel and Applications**
T M. Besmann, J Schorne-Pinto, M Aziziha, C M. Dixon, J Paz Soldan Palma, R E. Booth, A M. Mofrad, J A. Wilson (USC)
- 14:10 **Fission product chemistry and high temperature behaviour of irradiated MOX fuels with Pu/(U+Pu)=0.4**
C Gueneau, J-C Dumas, L Fayette (CEA)
- 14:30 *Afternoon coffee break*
- 14:50 **Progress in Coupling Computational Thermodynamics and Computational Fluid Dynamics: A Molten Salt Fast Reactor Application**
N L Scuro (OTU), O Benes (JRC) and M H.A. Piro (OTU)
- 15:10 **OECD/NEA TCOFF2 project: a proposed Systems Identification and Ranking Table (SIRT)**
C Journeau (CEA), S Bechta (KTH), M Kurata (JAEA), L Lovasz (GRS), H Esmaili (NRC), and A Dufresne (NEA)
- 15:30 Discussion
- 16:00 *Adjourn*

Dinner at Niagara Falls

- 17:00 *Bus to Niagara Falls – Pickup: Sheraton Hamilton Hotel, 116 King Street West, Hamilton, ON*
- 18:00 *Dinner at Table Rock Restaurant - 6650 Niagara River Pkwy, Niagara Falls*
- 20:30 *Bus return – Pickup: Table Rock Restaurant*

Thursday November 30th

- 8:50 *Arrival refreshments*
- 8:50 Announcements

Session D: Fuel performance

Chair: A. Prudil

- 9:00 **Approaches to Fission Product Chemistry Modelling in non-LWR Accident Analysis**
M S. Christian L I. Albright and D L. Luxat (SNL)
- 9:20 **Separate-Effects Irradiation Testing of Nuclear Fuels to Enhance Modelling and Simulation Accuracy**
J Gorton, N Capps, C Petrie, A Nelson (ORNL)
- 9:40 **Comparison of FAST Experiments to BISON Simulations**
A Swearingen, G L. Beausoleil, K Paaren, L Capriotti (INL)
- 10:00 Morning coffee break
- 10:20 **Towards designing fuel for a molten-salt cooled innovative AGR by means of TRANSURANUS**
A de Lara (UC), E Shwageraus (UC) and P van Uffelen (JRC)
- 10:40 **Overview for the Modelling of Defective CANDU Fuel Behaviour**
B. J. Lewis (RMC)
- 11:00 **Calibration of Fuel Performance Codes Addressing unknown uncertainty on calibration parameter**

G Robertson, H Sjöstrand, P Andersson, A Gööka (UU)

11:20 *Discussion*

Workshop wrap-up and farewell

Chair: M. Welland

11:40 *Discussion*

12:00 *Lunch to go*

13:00 **Tour of McMaster facilities**

Pickup: Sheraton Hamilton Hotel, 116 King Street West, Hamilton, ON

Affiliations:

CBU Cape Breton University, Canada
CEA Alternative Energies and Atomic Energy Commission, France
CINaM Centre Interdisciplinaire de Nanoscience de Marseille, France
DU Delft University of Technology, Netherlands
GE University Gustave Eiffel, France
KIT Karlsruhe Institute of Technology, Germany
KTH Royal Institute of Technology, Sweden
INL Idaho National Laboratory, USA
JAEA Japan Atomic Energy Agency, Japan
JRC European Commission, Joint Research Centre Karlsruhe
LANL Los Alamos National Laboratory, USA
MU McMaster University, Canada
NASA National Aeronautics and Space Administration, USA
NCSU North Carolina State University, USA
NEA Organisation for Economic Cooperation and Development, Nuclear Energy Agency
NRC National Research Council, USA
OPG Ontario Power Generation, Canada
ORNL Oak Ridge National Laboratory, USA
OSU Ohio State University, USA
OTU Ontario Tech University, Canada
PB Psiche Beamline, Synchrotron Soleil, France
PU Purdue University, USA
RMC Royal Military College, Canada
SNL Sandia National Laboratory, USA
ST Seaborg Technologies, Denmark
QU Queen's University, Canada
UC University of Cambridge, UK
UF University of Florida, USA
USC University of South Carolina, USA
USK University of Saskatchewan, Canada
UWM University of Wisconsin-Madison, USA
UU Uppsala University, Sweden

Posters

Flash talks: A succinct introduction to the poster and its presenter in order to attract attention.

- Presenters have 1 minute to introduce themselves and the topic of their poster.
- Optionally, you can send 1 slide to be sent to wpfm@oecd-nea.org to be preloaded and displayed during your introduction.

<p>Ab initio energetics and microstructural changes due to point defects and fission products in U3O8. J. I. Ranasinghe, B. Szpunar¹, J. A. Szpunar (U Saskatchewan)</p>
<p>Investigation of UO₂/α-Zr properties by atomistic simulations and crystallographic analysis M Qin, H Zhu, E Kuo, T Wei, and M Ionescu (ANSTO)</p>
<p>Phenomenological damage behavior of BWR pressure vessel by reaction between metal debris and structural materials T Sato, K Shimomura, Y Nagae (JAEA)</p>
<p>A Hybrid Rate Theory Model of Radiation-Induced Growth M Mohsini (QueenU), P Saidi(QueenU), L K. Béland(QueenU), Michael Welland (CNL), Mark R. Daymond (QueenU)</p>
<p>Crystal Plasticity Modeling of Hydride Precipitation in Zirconium Alloys M Taherijam, H Abdolvand (UWO)</p>
<p>Atomistic simulation of the structure, segregation and stability of grain boundaries in U-Zr fuel I Cheik Njifon, E Torres (CNL)</p>
<p>Modelling non-uniform nucleation of prismatic dislocation loops in zirconium alloys under irradiation P Saidi (CNL, QU), M Mohsini (QU), M Welland (CNL), M Daymond (QU)</p>
<p>A generalized approach to CALPHAD-informed multiphysics phase-field modelling and efficient quadratic implementation M.J. Welland (CNL). G. Karagozian (CNL, OnTechU)</p>
<p>Thermochemical Properties of Molten Fluoride Reactor Fuels with Iodine and Cesium J Schorne-Pinto, M Aziziha, C M. Dixon, and T M. Besmann (USC)</p>
<p>Studies of Aqueous Systems at Elevated Temperatures O Palazhchenko(OTU, UNB), G J. Francolini(OUT) and M H Kaye (OTU)</p>
<p>Recent Applications and On-going Developments of Thermochemica G Karagozian(CNL, OUT) , M. Poschmann(CNL, OUT), and M Piro (OTU)</p>
<p>Thermodynamic Surrogate Models and Thermodynamic Source Experimental/Ab-initio Database M Poschmann, M J. Welland, D Deng, A Trottier (CNL)</p>
<p>Thermal Modeling of Nuclear Fuel using Deep Learning and Finite Element Method N K Marimuthu and M Mkandawire (CBU)</p>
<p>Investigating material deficiencies in AGR 5/6/7 irradiated TRISO fuel using BISON P. Obreja, M.H.A. Piro (OTU)</p>
<p>Microstructural and thermal characterization of radial properties in mixed oxide (MOX) nuclear fuels J Ferrigno (OSU), T Pavlov (INL), F Cappia (INL), Marat Khafizov (OSU)</p>
<p>Simulating the performance of TRISO particles with XCT-derived geometries A. Prudil, R. Osmond, and M. Poschmann (CNL)</p>

