
Expert Group on Multiscale Modeling of Fuels (M2F)

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EGATFL-03 Task Force 1 Meeting

4th March 2015, Paris
**NSC activities**

**Nuclear Science Committee (NSC)**

- **Expert Group on Integral Experiments for Minor Actinide Management**
  - High Priority Request List for Nuclear Data
  - Methods and Issues for the Combined Use of Integral Experiments and Covariance Data
  - Co-ordinated Evaluation of $^{239}$Pu in the Resonance Region
  - Scattering Angular Distribution in the Fast Energy Range
  - Evaluation of Experimental Data in the Resolved Resonance Region

- **Working Party on International Nuclear Data Evaluation Co-operation (WPEC)**
  - Heavy Liquid Metal Technologies
  - Fuel Recycling Chemistry
  - Advanced Fuel Cycle Scenarios
  - Innovative Structural Materials
  - Innovative Fuels
  - Task Force on Benchmarking of Thermal-hydraulic Loop Models for Lead-alloy-cooled Advanced Nuclear Energy Systems

- **Working Party on Scientific Issues of the Fuel Cycle (WPFC)**
  - Advanced Monte Carlo Techniques
  - Criticality Safety Benchmarks
  - Burn-up Credit
  - Criticality Excursions
  - Assay Data of Spent Nuclear Fuel
  - Uncertainty Analyses for Criticality Safety Assessment

- **Working Party on Nuclear Criticality Safety (WPNCS)**
  - Reactor Physics and Advanced Nuclear Systems
  - Uncertainty Analysis in Modelling
  - Reactor Fuel Performance
  - Radiation Transport and Shielding

  - Validation and Benchmarks of Methods
  - Multi-scale Modelling Methods
  - Structural Materials Modelling
  - Multi-scale Modelling of Fuels
  - Primary Radiation Damage

- **Executive Group of the NSC (Data Bank Management Committee)**
  - Databases and Scientific Services
  - The Scientific Co-ordination Group of the Joint Evaluated Fission and Fusion (JEFF) Data Project

- **Expert Group on Accident Tolerant Fuels**

- **Expert Group on MP Experimental Data, Benchmarking and Validation**

04/03/2015

EGATFL-03 Task Force 1 Meeting
NSC activities related to fuels

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- Working Party on Reactor Systems (WPRS)
  - Reactor Physics and Advanced Nuclear Systems
  - Uncertainty Analysis in Modelling
  - Reactor Fuel Performance, Radiation Transport and Shielding

Executive Group of the NSC (Data Bank Management Committee)

- Databases and Scientific Services

The Scientific Co-ordination Group of the Joint Evaluated Fission and Fusion (JEFF) Data Project

Thermodynamics of Advanced Fuels International Database (TAF-ID)

Expert Group on Accident Tolerant Fuels

Expert Group on MP Experimental Data, Benchmarking and Validation
NSC activities related to fuels and structural materials

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**Expert Group on Accident Tolerant Fuels**

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**Thermodynamics of Advanced Fuels International Database (TAF-ID)**
NSC material-related activities presented at EGATFL-03

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**Thermodynamics of Advanced Fuels International Database (TAF-ID)**
Outline

• Working Party on Multiscale Modelling of Fuels and Structural Materials (WPMM)
  ❑ Expert Group on Multiscale Modelling of Fuels (EGM2F)
  ❑ Overview of Multiscale Modelling Methods EG (M3)
  ❑ Overview of Structural Materials Modelling EG (SMM)
  ❑ Overview of Primary Radiation Damage EG (PRD)
  ❑ Overview of Task Force on Mechanisms of gaseous FP release

• Expert Group on Reactor Fuel Performance and IFPE Database (see next presentation)
WPMM scope

Set up in 2008, renewed mandate 2014-2016

- Focused on materials science aspects of nuclear fuels and structural materials

- Aims at promoting and developing multiscale models and simulations as validated predictive tools for nuclear fuel design, fabrication and performance
Structure of the WPMM Expert Groups (2009 – 2014)

WPMM
Multi-scale Modelling of Fuels and Structural Materials for Nuclear Systems

PRD
Primary radiation damage
EXPERT GROUP

State-of-the-art modelling

VBM
Validation and benchmarking
EXPERT GROUP

M3
Multi-scale modelling methods
EXPERT GROUP

M2F
Multi-scale modelling of fuels
EXPERT GROUP

SMM
Structural materials modelling
EXPERT GROUP

WPMM
Multi-scale Modelling of Fuels and Structural Materials for Nuclear Systems

State-of-the-art modelling

M3
Multi-scale modelling methods
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Structural materials modelling
EXPERT GROUP

Renewed mandate (2014-17)
- VBM merged with M3
- PRD completed its activity

WPMM
Multi-scale Modelling of Fuels and Structural Materials for Nuclear Systems

- **Task Force related to Structural Materials Modelling**
  - *(will be established in 2015)*

- **Task Force on ‘Unit Mechanisms of gaseous FP release’**

  - **M3**
    - Multi-scale modelling methods
    - EXPERT GROUP

  - **M2F**
    - Multi-scale modelling of fuels
    - EXPERT GROUP

  - **SMM**
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Multi-scale Modelling of Fuels and Structural Materials for Nuclear Systems

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Task Force on ‘Unit Mechanisms of gaseous FP release’

M3
Multi-scale modelling methods
EXPERT GROUP

M2F
Multi-scale modelling of fuels
EXPERT GROUP

SMM
Structural materials modelling
EXPERT GROUP
EG M2F objectives

- Assess **multiscale modeling approaches** devoted to nuclear fuels from the atomic to the macroscopic scale in order to share and promote such approaches.

- Address **all types of fuels**: current (mainly oxides) and advanced (oxide, carbide, nitride, metallic fuels, fuels with minor actinides).

- Foster **integration** of results from multi-scale modeling and simulation into performance codes.

- Assess the quality of existing **links between the various scales** and list needs for strengthening multi-scale modeling approaches.

- Promote exchange between multiscale modeling experts and **experimentalists**.
EG M2F objectives

- Identify the most relevant experimental data or experimental characterization techniques that are missing for validation of fuel multiscale modeling

- Address key engineering issues associated with each type of fuels, for which combining modeling and experiment could contribute to reducing the time and resources needed to develop/improve fuels

  ➔ Set up of Task Forces

- Foster international cooperation on multiscale modeling of nuclear fuels by sharing state-of-the-art models, expertise, progress and key issues in multiscale modeling
Computational Approaches: Practicing Engineer

From S. Phillpot (Univ. Florida), OECD-NEA NSC Meeting, 13/06/14 (figure adapted from Marius Stan, DOE)
Computational Approaches: \(~1985\)

From S. Phillpot (Univ. Florida), OECD-NEA NSC Meeting, 13/06/14 (figure adapted from Marius Stan, DOE)
Computational Approaches: 2015

From S. Phillpot (Univ. Florida), OECD-NEA NSC Meeting, 13/06/14 (figure adapted from Marius Stan, DOE)
EG M2F deliverable

State-of-the-art report on fuel multi-scale modeling approaches, including:

- **Key engineering issues** that are relevant for the various fuels

- A worldwide **state-of-the-art review** of modeling approaches, from the atomic scale (first-principles and empirical potentials methods) to the macroscopic scale (fuel performance codes)

- A focus on **mid-term and long-term challenges** for the future (approximations, methods, scales, key experimental data, characterization techniques missing or to be strengthened)

*Draft version available since October 2013, reviewed in 2014, final version currently being edited, the report will be published in April 2015*
Part I: Underlying phenomena of nuclear fuel behavior

A complex behavior: numerous coupled phenomena and interconnected effects

- Cracking
- Fission gas bubble precipitation
- High Burn up structure
- Radial migration
- FP migration / interaction

Microstructure changes under irradiation, Mechanical behaviour, Thermodynamic stability / chemical interaction, Thermal Transport
Part I : Underlying phenomena of nuclear fuel behavior

- **I.01** Microstructural changes of fuel under irradiation
  Radiation damage, fission gas bubble formation, high burn-up effects, …

- **I.02** Nuclear fuel deformation
  Creep, swelling, cracking, pellet-clad interaction
  L. Van Brutzel, R. Dingreville, T. Bartel

- **I.03** Chemical interactions
  Fuel/cladding, fuel/coolant, cladding/coolant chemical interactions
  C. Guéneau, J. Piron, J-C. Dumas, V. Bouineau, B.J. Lewis, F.C. Iglesias, C. Desgranges, C. Toffolon

- **I.04** Property / process relationships in fuel fabrication
  Microstructure, porosity, density optimisation, …
  V. Tikare

- **I.05** Phenomena in thermal transport in fuels
  Phonons / radiation damage interactions, conductivity models…
  A. Chernatynskiu, A. El-Azab, J. Tulenko, S. Phillpot
Part II: Methodologies for determining nuclear fuel properties

- **II.01** Theoretical estimation of thermal expansion of nuclear fuels
  - Y. Yun

- **II.02** Atomic transport properties
  - M. Freyss

- **II.03** Free energy and heat capacity
  - M. Kurata, R. Devanathan

- **II.04** Elastic and viscoplastic properties
  - R. Lebensohn
Part III: Principles of modeling techniques for fuels

- **III.01** Density Functional Theory - M. Freyss
- **III.02** Classical Molecular Dynamics - R. Devanathan, M. Krack, M. Bertolus
- **III.03** Dislocation Dynamics - L. Van Brutzel
- **III.04** Assessment of atomic scale modeling methods for UO$_2$ - M. Bertolus, M. Freyss, M. Krack, R. Devanathan
- **III.05** Phase Field - B. Radhakrishnan, S.B. Gorti, K. Clarno, M. Tonks
- **III.06** Peridynamics – D. Littlewood
- **III.07** Kinetic Monte Carlo - V. Tikare
- **III.08** Rate Theory - S. Maillard, R. Skorek, P. Maugis, M. Dumont
- **III.09** Thermochemical Modeling - B. Sundman, C. Guéneau
- **III.10** Viscoplastic Models - R. Masson, V. Blanc, J.M. Gatt, J. Julien, R. Largenton, B. Michel
- **III.11** Finite Element Modeling - M. Tonks, R. Williamson, R. Masson
- **III.12** Integration/Multiscale – C. Valot, L. Malerba
- **III.13** Fuel Performance Codes - P. Van Uffelen

WPMM
Multi-scale Modelling of Fuels and Structural Materials for Nuclear Systems

Task Force related to Structural Materials Modelling
(will be established in 2015)

Task Force on ‘Unit Mechanisms of gaseous FP release’

M3
Multi-scale modelling methods
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EG on Multiscale Modelling Methods (M3)

Objective: assess the possibilities and limits of both numerical methods applied to multi-scale modelling of materials for nuclear energy and means to link them

- Outline of the methods as applied to nuclear materials
- Advantages & disadvantages
- Limits, needs & recommendations
- Foster exchange of experience and dissemination of knowledge

- Chair: V. Tikare (SNL, USA)
- Vice-Ch.: M. Crack (PSI, Switzerland)
EG on Structural Materials Modelling (SMM)

- New Chair: P. Olsson, (KTH, Sweden)
- Vice-Ch.: L. Malerba (SCK-CEN, Belgium)

- Invented to allow the investigation of phenomena that cannot be studied experimentally - ideally *ab initio*
- Should be able to reproduce / predict how the nanostructure and the microchemistry changes under irradiation
- Should be able to reproduce / predict changes of mech. ppties under irradiation
EG on Primary Radiation Damage (PRD)

Objectives:
- to assess the limitations of the NRT-dpa standard
- to revisit the NRT-dpa standard and examine the possibility of proposing a new improved standard of primary damage characteristics.

Objective:

The final report will be published in March 2015 on the NEA website.
Task Force on “Unit mechanisms of gaseous FP release”

- Established in 2014 between 12 experts, coordinated by M. Tonks (INL, USA)

- Scope: **summarizing existing research** on the basic mechanisms behind the various stages of fission gas release during normal reactor operation and **identify critical areas** where experimental and simulation work is needed
  - Identify fission gas behaviour mechanisms
  - Determine critical modelling parameters
  - Relate model parameters to physics-based phenomena
  - Critically assess existing data
  - Recommend new, key experiments/simulations

  - First draft scheduled for mid-2015
  - Final report scheduled mid-2016