"Materials Modeling and Simulations for Nuclear Fuels" Workshop
November 20-21, 2003, New Orleans, LA

Summary of the Workshop

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The workshop was organized as part of the Advanced Fuel Cycle Initiative (AFCI) program, addressing the area of predictive fuel performance. The members of the organizing committee: M. Stan (LANL), J. Tulenko (Univ. Florida), K. Chidester (LANL), Robin Grimes (Imperial College, London, UK), and K. McClellan (LANL) as well as K. Pasamehmetoglu (National Director for Fuels Program) and E. Arthur (NTA office) joined efforts in preparing the technical program and advertising the workshop.

Forty participants attended the meeting, representing Belgium, Germany, Japan, the Netherlands, Sweden, United Kingdom, and the United States of America. Participants from six USA National Laboratories (Argonne, Idaho, Lawrence Livermore, Los Alamos, Oak Ridge, and Pacific Northwest) were present. The lone area showing a decrease in attendance from the first workshop was university participation. There was one participant from the industry/private companies. More participation by Industry and Universities will be sought for future meetings in order to have a truly balanced attendance.

The committee thanks Rose Romero (Conference Coordinator) and Lynne Johnson (Webmaster) for their contribution and constant help. For additional information on the workshop, please visit: http://www.lanl.gov/orgs/mst/mmsnf/

The second edition of the workshop shifted the focus of the discussions from materials science to fuel performance predicative codes. The presentations were grouped in three Technical Sessions: *Fuel Performance Codes* (Thursday, Nov. 20, afternoon), *Modeling and Simulations* (Friday, Nov. 21, morning), and *The Impact of Modeling, Simulations, and Fuel Codes on Nuclear Fuels Development* (Friday, Nov. 21, afternoon). The 20 min. talks of sessions A and B were followed by a plenary discussion of the session's subject. The workshop ended with a plenary discussion during session C. A summary of the discussions is presented below. Some presentations are discussed in the session that best fits their content rather than the actual technical program session. For a detailed agenda, please see the web page. Copies of the presentations, on CD-ROM, are available by contacting Marius Stan (mastan@lanl.gov).

The organizing committee thanks all participants for their contribution to the success of the workshop. The notes below are based on the discussions during the workshop. Thanks to Paul Van Uffelen and all other participants who contributed with comments.

A) Fuel Performance Codes (Chair K. Chidester)

K. Pasamehmetoglu (LANL, USA) Advanced Fuel Cycle Initiative Requirements for Modeling and Fuel Codes.

D.D. Lanning (PNNL, USA), *et al.* Review of FRAPCON and FRAPTRAN Fuel Performance Codes.

P. Van Uffelen (ITU, Germany) The TRANSURANUS Fuel Performance Code: Present Status and Future Developments.

D. Petti (INEEL, USA), *et al.* Coated Particle Fuel Modeling Using the PARFUME Code.

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M. K. Meyer (ANL, USA), *et al.* Fuel Performance Modeling for Metallic and Dispersion Actinide Transmutation Fuels.

H. Aït Abderrahim (SCK·CEN, Belgium) Modelling Behaviour of Prototypic (Am,Pu)O2 Targets with ZrO2 and ThO2 Matrices in a Small Experimental ADS MYRRHA.

J. S. Choi (LLNL, USA), *et al.* Computational Evaluation of Nitride-Based Fuel Performance.

J. Rashid (ANATECH) Nuclear Fuels Modeling with FALCON.

The following codes were either reviewed, discussed, or mentioned as being relevant:
COMETHE (Belgonucleaire, Belgium)
COPERNIC (FRAMATOME, Germany)
ENIGMA (British Energy, BNFL, UK)
FALCON (EPRI, USA)
FRAPCON (PNNL, USA)
FRAPTRAN (PNNL, USA)
LIFE (ANL, USA)
MACROS (SCK-CEN, Belgium)
MCNPX (LANL, USA)
ORIGEN (ORNL, USA)
PARFUME (INEEL, USA)
SPHERE (PSI, Switzerland)
TRANSURANUS (ITU, Germany)
TRUCHAS (TELLURIDE)

Discussion items:

1. Several codes account for grain growth (normal and columnar), central void formation (FBR fuel) and some account (empirically) for the high burnup structure.
2. The microstructural evolution (detailed modeling of point defects and dislocations along with grain boundary movement) during service is not present in any fuel performance code. Truchas (casting simulation software) is an example of a code able to address that area.
3. Heat transfer simulations based on thermal conductivity models must provide input for the fuel codes.
4. The thermo-chemistry of chemical reactions, such as oxidation/reduction must be included. TRANSURANUS accounts for radial redistribution of oxygen in FBR fuel.
5. Thermo-mechanical properties and phenomena, such as:
    - enthalpy
    - heat capacity
    - thermal conductivity
    - thermal expansion coefficients
    - dislocations
    - fracture
    - swelling
    - void formation

must be modeled as a function of

- temperature
- pressure

- non-stoichiometry
- porosity
- irradiation
- burn-up
- etc.

6. The interpolation and extrapolation of models is difficult when using correlations. In order to make predictions for new fuel types there is a need to develop more physically based codes. This has become possible with the advances in computation capabilities along with more detailed experimental techniques.
7. There is a need for better physics in most codes. The correlations are too empirical.
8. The codes are too fuel specific. It is difficult to extend their use to new fuel types.

B) Modeling and Simulations of Materials Properties (Chair J. Tulenko)

K. Minato (JAERI, Japan) A Review of the Modeling and Simulations for Nuclear Fuels at JAERI.

J. M Wills (LANL, USA), *et al.* Elastic and Thermodynamic Properties of Transition-Metal and Actinide Nitride Compounds.

C.R. Stanek (LANL, USA), *et al.* Segregation of Fission Products to Surfaces of UO2.

D. Price (AWE, UK) Molecular Modelling Studies of Transport Phenomena in UO2.

J. Wallenius (KTH, Sweden) In-and out of Pile Modelling of Cr Precipitation in Fe-Cr Alloys.

B. P Uberuaga (LANL, USA), *et al.* Molecular Dynamics, Molecular Statics, and Temperature Accelerated Dynamics Study of Radiation Damage Events and Subsequent Annealing in MgO.

R. C. Martin (ORNL) Nuclear Fuels at ORNL.

M. Stan (LANL, USA), *et al.* Phase Stability and Diffusion in Actinide Based Ceramics and Surrogate Materials.

F.C. Klaassen (EC, The Neatherlands), *et al.* Boron Implantation to Study Minor Actinide Transmutation (BISMAT); A Quick Tool to Assess Alpha Decay Damage in Inert Matrices.

Discussion Items:

9. All types of fuels must be studied: oxides, nitrides, metallic, dispersed (inert matrix), composite and carbides, as possible fuel types.
10. Modeling and Simulations must address all scales, starting with the nucleus, the electronic structure, atomistic and nano-scale, mezzo-scale, all the way to the continuum level properties and phenomena.
11. The modeling and simulation results must feed into the fuel codes.
12. The experimental testing and actual performance results must feed into the fuel codes.
13. Creep is a critical property that must be modeled in detail. The simulation of fuel creep is most important phenomena. "If we knew creep we know everything".
14. Understanding of the fuel structure (grain size, porosity and chemistry) and the behavior under irradiation and temperature are a priority.
15. Studies of the particular aspects of the fission process and fuel fission products that affect materials properties are required.
16. For metallic fuels, complete multi-component phase diagrams are important.
17. For ceramic fuels, pseudo-binary diagrams are a priority.

18. The electronic structure calculations must go up in temperature. Results at finite temperatures are required.
19. Accelerated Molecular Dynamics (MD) or combinations of MD and Mont Carlo simulations can describe times of the order of micro-seconds, specific for diffusion of species.
20. Non-equilibrium phenomena, such as quenching, should be given priority.
21. The computational resources and the computational time have prevented scientists from running complex simulations on millions of atoms to address bulk properties. That computational activity requires better computers and international collaboration. As computers have improved, these calculations have become more feasible

C) The Impact of Modeling, Simulations, and Fuel Codes on Nuclear Fuels Development
(Chairs J. Tulenko and M. Stan)
J. Wallenius (KTH) Recent Modeling Results at KTH.
L. J. Ott (ORNL) Overview of Modeling Needs for Oxide Fuels.
J. Rashid (ANATECH) The Future of Nuclear Fuels Modeling and Simulations.
M. Stan (LANL) Simulation Scales and Methods

22. It is well understood that empirical modeling is valuable, but is limited in applicability and is essentially only valid within the confines of parameters and irradiation conditions covered in the database on which it is developed.
23. There are areas where first principle or atomistic models can be developed to better understand the important mechanisms contributing to critical phenomena.
24. The modeling of nitride fuels is more advanced in Europe and Japan. US research must accelerate the modeling effort.
25. A smaller group must work on prioritizing the areas.
26. We have to team up in developing complex software packages.
27. Compatibility is critical for merging various pieces of software.
28. The models must be validated through experimental work.
29. There is a need for a comprehensive plan, to allow for both short-tem and long term activities.
30. The funding of modeling and simulation must increase.
31. Modeling and simulations can contribute to the fuel qualification process.
32. The following have been mentioned as important areas:
    - Fuel structure (grain size, porosity and chemistry) behavior under irradiation and temperature
    - Fission gas release, diffusion, and location
    - Fission products release, diffusion, and location
    - Fuel densification and swelling
    - Thermal performance and calculating fuel temperatures
    - Fuel creep
    - Pellet fragmentation and relocation
    - Thermo-mechanical interactions of pellets with clad
    - Clad behavior (oxidation, hydrating, creep, mechanical, water chemistry, etc)
    - Gap composition and geometry

D) Collaboration and Future Workshops

33. The first action resulting from the 2nd workshop was to identify specific aspects of fuel behavior and potential reviewers to appraise the current state of understanding in those areas and have these discussed at the 3rd workshop.
34. Modeling and simulation sessions at both the winter and the summer ANS meetings are desirable. There are placeholders for the next two meetings.
35. Workshops will be also coupled with the ANS meetings, to allow for discussions and debate.
36. The 3rd Workshop must focus on explicit areas such as:
37. fuel conductivity modeling
38. fuel clad-gap evolution modeling
39. fission gas modeling
40. It is proposed that an international consortium be organized and a program be designed to develop a coherent set of computer programs to simulate fuel behavior under normal operating conditions, with extension to abnormal conditions.