Neutronics, nuclear fuel and burnup (NEPAL)

Aalto University
School of Science
Dept of Applied Physics
Fission and Radiation Physics
Project manager: DSc (Tech) Jarmo Ala-Heikkilä

SAFIR2014 mid-term seminar / 21.-22.3.2013
Project organization

**Scientific staff:**
- Research associate: MSc (Tech) Aarno Isotalo
- Research associate: MSc Markus Ovaska
- Research assistant: BSc (Tech) Antti Rintala
- Research assistant: MSc (Tech) Ville Valtavirta
- Research associate: MSc (Tech) Risto Vanhanen

**Project management:**
- Project manager: DSc (Tech) Jarmo Ala-Heikkilä
- Deputy manager: DSc (Tech) Seppo Sipilä

**Internal reference group:**
- Prof. Rainer Salomaa
- DSc (Tech) Pertti Aarnio
- Prof. Mikko Alava
- Prof. Filip Tuomisto
Project goals 2011-2014

- Development of methodology of Monte Carlo codes
- Improving speed and accuracy of MC-codes
- Coupling the temperature distribution of fuel to neutronics
- Accurate burnup calculations
- Mesoscopic modeling of nuclear fuel
- Preparations for new international projects (JHR…)

- Main deliverable: Education of new experts!
NEPAL subtasks in 2011-2012

1. Development of accurate methods for burnup calculations
   - Platform: Serpent
   - Researchers: Isotalo, Vanhanen

2. Coupling the temperature distribution of fuel to neutronics
   - Platform: Serpent
   - Researchers: Valtavirta, Rintala

3. Mesoscopic modeling of nuclear fuel: thermal creep and fission gas diffusion
   - Platform: new code (still unnamed)
   - Researcher: Ovaska

The fruitful collaboration with the KÄÄRME and PALAMA projects of VTT in area 3 is acknowledged. (Remember to visit the poster of KÄÄRME!)
Development of accurate methods for burnup calculations (subtask 1)

- **What?** Follow *time development of material compositions* and *neutronics* when nuclear fuel is irradiated.

- **How?** Combine sequential steady state neutronics (flux etc.) and depletion (material changes) solutions.

- **New?**
  - Better burnup algorithms: *Higher order methods* and *substeps*.
  - *Damping xenon oscillations*.

- **Why?**
  - Calculations in large geometries feasible.
  - More accurate or faster (via longer steps) calculations.

- **Generic?** Yes, but Serpent has been used as testing platform.
New burnup algorithms: example test case

Westinghouse 17x17 PWR assembly

16 poison rods with 3% natural Gd

Periodic boundary conditions
Specific power: 38.6 kW/kgHM
Final burnup: 40 MWd/kgHM
Enrichment: 4.2 atom-%
Boric acid: 760 ppm
Element size: 21.6 cm
New burnup algorithms: example results

Absolute and relative errors in Gd-155 atomic density as a function of burnup

Colors: different order combinations

Dashed: with substeps

Absolute error in $k_{\text{eff}}$ as a function of burnup

Colors: different order combinations

Dashed: with substeps
New burnup algorithms: example results

Relative error in U-235 atomic density as a function of burnup
Colors: different order combinations
Dashed: with substeps

Relative error in Sm-149 atomic density as a function of burnup
Colors: different order combinations
Dashed: with substeps
Xenon stability (1)

- Xenon driven oscillations in large geometries
  - Prior studies by others: All existing methods affected
  - Effectively prevents calculations with large and detailed geometries
- 15 min steps $\rightarrow$ physical xenon oscillations
- The model describes physical oscillations, not secular equilibrium
  - The problem is in the model, not the algorithms

Flux and xenon concentration in segment 1 with a small enrichment difference and 15 min steps. Four runs with different random number sequences.
Xenon stability (2)

- Solution: change the model by requiring that flux and xenon must remain in equilibrium
- Efficient calculation via integrated equilibrium algorithms
  - Such algorithms already exist (developed for other purposes)
- Depletion driven oscillations still arise with >= 60d steps

NOTE: Without equilibrium xenon oscillations happen between predictor and corrector => results look stable but are wrong
Conclusions of subtask 1

- Higher predictor order has clear positive effect in assembly geometries
- Higher corrector order has not, but might still be preferable due to predictability
- Substeps have large effect with long steps and on short lived nuclides
  - Complements higher order methods
- Xenon stability problems in Monte Carlo burnup calculations reflect instability of the simulation model, not the solution algorithms
  - **Solution: force xenon and flux to equilibrium**
  - Efficient with integrated equilibrium algorithms
Coupling the temperature distribution of fuel to neutronics (subtask 2)

- **Goal?** Combine Monte Carlo neutronics with thermal hydraulic codes
- **Problem?** Cross sections in neutronics depend on temperature; fuel temperature is typically discretized
- **Solution?** An internal fuel element temperature solver routine, now implemented in fresh 2D pin-geometries (enhancements later)
- **Generic?** Yes but Serpent has been used as the testing platform for practical reasons
- **Why?** In order to reach a more realistic model of the reactor core and to reduce errors from approximations
Temperature discretization: simulations

- A pin-cell with 30 fuel rings of eq.vol + gas + cladding.
- External coupling to a temperature solver.
- Volume averaging of temperatures in each ring.
- The number of temperature zones reduced to 1, 2, 4, 8, 16 or 24.
- Reference was 32 temperature zones \((\approx)\) accurate.
- Depletion calculation until 60 MWd/kgU.
- Comparison of nuclide compositions & reactivities.
- Averaging over 10 depletion calculations.
Temperature discretization: case Pu-239

**Pu-239 concentrations**

*Left:* Radial mass fractions at different burnups

*Right:* Relative errors with different numbers of temperature zones

(Mean temperature and number of depletion zones are equal)
Temperature discretization effects on $k_{\text{eff}}$
Conclusions of subtask 2

• Serpent was coupled to an external fuel temperature solver
• Depletion calculations were performed with different radial temperature discretizations
• **Local and total errors in nuclide composition** resulting from inaccurate radial temperature discretization were estimated
  – Inaccurate discretizations tend to overpredict the produced amounts of the followed fission products and actinides
  – A higher amount of the fission power is generated in Pu-239 fissions when inaccurate discretizations are used
  – Differences halved when the number of temperature zones doubled
Mesoscopic modeling of fuel: thermal creep and fission gas diffusion (subtask 3)

- Background? **Structure and properties of nuclear fuel change significantly during reactor operation**
- Goal? Model the basic physical phenomena: formation of bubbles, radiation damage, fission gas diffusion, thermal creep
- How? Start from a simplistic model and add features
- Method? Utilize **percolation theory** where gas flows through interlinked pores, and a **fuse model** for radiation damage
- Generic? Yes, starting from the basic phenomena
- Why? In order to better understand the observed behavior of nuclear fuel
Nuclear fuel characteristics

- Fission gas diffusion interlinked with microstructural evolution of fuel pellet
- Thermal stresses cause radial fragmentation and microcracking
- Fission gas bubbles form within the pellet
- Increasing porosity of fuel enhances gas diffusion

SAFIR2014 mid-term seminar / 21.-22.3.2013
Microfracture modeling

- Model a pellet under constant thermal stress: creep
- Discrete scalar model
- **Creep fracture** in damage mechanics: Young's modulus of bonds is decreased: $E \rightarrow (1-d)E$
- Stress-strain relation: $\sigma = E(d)\varepsilon$
- Connection between damage and porosity in nuclear fuel e.g. from ultrasonic testing


Gas release and concentration profiles

Release rate:

Steady state concentrations:

Total released gas:
Conclusions of subtask 3

• Thermal creep fracture and radiation damage change porosity of fuel pellet
• Diffusion of fission gas strongly affected by local porosity: above or below percolation threshold?
• Percolation threshold depends on shape and distribution of pores: gas bubbles and microcracks
• A model for gas diffusion and thermal creep: diffusion coefficient depends locally on accumulated damage
• Further developments:
  – Time evolution of porosity during gas diffusion
  – Explicit dependence between porosity and gas concentration
  – Percolation threshold from different pore distributions
Conclusion

Research on neutronics, nuclear fuel and burnup continues. New doctors, masters and bachelors are being educated.

Thank you for your attention!
References