Multiscale modeling of fission gas behavior for BISON

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Outline

- BISON fuel performance code
- Fission gas model for UO$_2$
- Examples of validation results
- Lower-length scale modeling for the parameters
- Multiscale fission gas model for U$_3$Si$_2$
- Outlook
- Acknowledgements
**BISON fuel performance code**

- Finite element based, engineering fuel performance code based on INL’s open-source MOOSE framework
- Solution of fully-coupled equations of thermo-mechanics in 1D, 2D, or full 3D
- Used to analyze various fuel forms including LWR, TRISO, and fast metal and oxide fuels
- Designed for efficient use on parallel computers

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Stages of fission gas behavior

1. **Fission reactions**
   - Generation of fission gases (Xe, Kr)

2. **Intra-granular gas** (single atoms)
   - Diffusion
   - Trapping
   - Resolution

3. **Intra-granular gas** (bubbles)
   - Diffusion

4. **Grain-boundary gas**
   - Diffusion

5. **Grain-boundary bubble swelling**

6. **Saturation / Micro-cracking**

7. **Fission gas release**
Intra-granular model

- Computes intra-granular bubble evolution and swelling, and gas diffusion to grain boundaries
- Derived from cluster dynamics equations, simplified for application to engineering codes
- Can be informed with improved parameters from advanced lower-length scale models

\[
\frac{\partial N}{\partial t} = +v - \alpha_n N
\]

\[
\frac{\partial m}{\partial t} = +2v + \beta_n N - \alpha_n m
\]

\[
\frac{\partial c_1}{\partial t} = +yF + D\nabla^2 c_1 - 2v - \beta_n N + \alpha_n m
\]

Grain-boundary model

- Bubble growth with inflow of atoms and vacancies (Speight and Beere, Met. Sci. 9, 1975)

\[ \frac{dn_v}{dt} = \frac{2\pi D_v \delta_g}{kTs} (p - p_{eq}) \]

- Bubble coalescence with geometrical reasoning (White, JNM 325, 61-77, 2004)

- Gaseous swelling coupled to FGR

- Two FGR contributions:
  - Grain-boundary saturation
    \[ \frac{dF_c}{dt} = \frac{d(N_{gr}A_{gf})}{dt} = 0 \quad \text{if} \quad F_c = F_{c,\text{sat}} \]
  - Burst release associated with micro-cracking


Separate-effects validation examples

Comparisons of local grain-boundary swelling in power-ramped UO$_2$ (Pastore et al., NED 256, 2013). Experimental data from White et al., R&T/NG/EXT/REP/0206/02, 2006.

Integral validation examples

**Risø-3 AN4**

Integral FGR vs time during LWR fuel rod power ramp experiment (Risø-3 AN4)

Integral FGR at EOL for 19 LWR fuel rod power ramp experiments
Integral validation examples

Radial profiles of Xe concentration after ramp tests calculated with BISON and PIE data
CABRI REP Na-3 power pulse test

Left: Power, calculated energy deposited and radially averaged fuel enthalpy at peak power node

Right: FGR with fuel centerline temperature. The inset shows a shorter time around the power pulse
CABRI REP Na-3 power pulse test


Right: FGR with fuel centerline temperature. The inset shows a shorter time around the power pulse
Atomistic modeling for Xe diffusivity

- Atomistic (DFT, empirical potential) modeling for the diffusivity of Xe in the UO$_2$ matrix is performed at Los Alamos National Lab.
- Early work led to a new diffusivity model that was implemented in BISON (D.A. Andersson et al., JNM 451, 225, 2014)
- Further work is in progress at LANL
Atomistic modeling for Xe resolution

- Molecular dynamics (MD) calculations for the Xe resolution rate from intra-granular bubbles were performed at Pacific Northwest National Lab. (W. Setyawan et al., in preparation)
- Will be used to inform the engineering model in BISON
Phase-field modeling for grain-boundary saturation

- Phase-field model of bubble evolution at grain faces and edges (triple junctions) was developed at INL.
- Grain-edge coverage and saturation was correlated to grain-face coverage.
- Can be used to inform the engineering model with thresholds for FGR from the grain edges.

Tucker, Radiation Effects, 53, 1980
Multiscale fission gas model for $\text{U}_3\text{Si}_2$

- Initial model of fission gas behavior in $\text{U}_3\text{Si}_2$ for BISON
- Informed by atomistic calculations for the basic parameters (resolution, diffusivity), to fill the experimental data gap
- Sensitivity analysis to help addressing future research

![Shimizu, Report NAA-SR-1062, 1965](image)

### Figure 3.2
Re-solution parameter calculation for several fuel types using the values in Table 3.1.

$\text{U}_3\text{Si}_2\text{r} = 10.0$ g/cm$^3$

$\text{U}_3\text{Si}_2\text{r} = 10.0$ g/cm$^3$

$\text{U}_3\text{Si}_5\text{r} = 10.0$ g/cm$^3$

$\text{U}_3\text{Si}_2\text{r} = 12.2$ g/cm$^3$

### Figure 3.3
Re-solution parameter calculation for different silicide fuels with the exact same density of 10 g/cm$^3$.

C. Matthews, D. Andersson, C. Unal, LANL, 2016)
Outlook

- Inform BISON fission gas models with new parameters from atomistic models of Xe diffusion and resolution
- Extend intra-granular model to bubble coarsening and the associated fuel swelling during transients/high burnup
- Extend fission gas model to gaseous porosity evolution in the high burnup structure (HBS)
- Continued model validation
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