PROGRESS IN MODELLING FISSION-PRODUCT RELEASE: AN UPDATE WITH RESPECT TO IRSN’S RELEASE CODES

R. Dubourg, M.P. Kissane , P. Taylor, W. Plumecocq

www.irsn.org
Outline

1. Context
2. Improvement of ASTEC/ELSA
3. Improvement of MFPR
4. Conclusions
Context

- Two codes developed, different objectives...
- ELSA, part of integral ASTEC code, semi-empirical tool for reliable and rapid calculation of release of all FPs, actinides and structural materials from degrading cores for all LWR SA core configurations
- MFPR, developed with the Nuclear Safety Institute of the Russian Academy of Science, highly-mechanistic approach modelling grain-scale and sub-grain phenomena for insight into state of fuel and FPs for all transients, SA or otherwise
- Both codes presented in some detail 2 years ago
Improvement of ASTEC/ELSA

- Validation studies (e.g., ISP-46) showed deficiencies in two key areas
  - Release of so-called semi-volatile FPs, Ba, Mo, Ru, etc.
    - significant improvement required:
      can contribute substantially to the source term;
      major role in core degradation via decay heating
  - Release of structural elements
    - improvement for Ag-In-Cd control rods:
      impact on downstream chemistry, esp. iodine
    - addition of other alloys, Cr, Fe, Nb, Ni, Sn (urgent), Zr:
      impact on downstream chemistry + high aerosol source
Improvement of ASTEC/ELSA

- Release of semi-volatile FPs where chemistry determines evaporation from UO$_{2+x}$ or precipitate phase
  - Speciation of 8 FPs reassessed using mainly GEMINI 2 (Thermodata-IRSN) + FACT-web, MFPR database, report AECL-9552
  - Total pressure $P_M = \gamma_{MOq} \cdot x_{MOq} \cdot \sum_{1}^{n} P_{MOxHy}$
    - $\gamma_{MOq}$ activity coeff.
    - $x_{MOq}$ mole fraction in solid solution (Raoult)
    - $P_{MOxHy}$ species vapour pressure
  - Evaporating species: Sr, La, Ce, Eu as M + MO;
    - Ba as Ba + BaO + empirical treatment;
    - Ru as Ru + 4 oxides, separate phase;
    - Mo as Cs$_2$MoO$_4$ + empirical treatment;
    - Y re-classed as non-volatile
Improvement of ASTEC/ELSA

- Release of structural elements
  - Require chromium, iron, niobium, nickel, tin and zirconium, tin highest priority
  - Correlation between Zrly oxidation and Sn release, e.g., Phébus FPT1, linearly proportional with factor 0.6
  - Requires confirmation in reducing conditions
Improvement of ASTEC/ELSA

- Release of structural elements
  - Ag-In-Cd improvement: mass transfer at surface dealt with as for molten pool of corium; progression fixed by $\text{Fe}_3\text{O}_4$ melting (canister partially oxidized)
  - In overestimated: chemistry ($\text{In, In}_2\text{O, InOH, In}_2\text{O}_3$)?
  - Pursued in SARNET
Improvement of MFPR

- Evolution of the code to treat more than just SAs
  - Both SA and especially design-basis LOCAs affected by pre-transient state of fuel, i.e., evolution during irradiation regime
  - Improvements relate mainly to fission gases & modelling of irradiation-regime phenomena for higher burn-ups:
    - point-defect evolution (vacancies, interstitials, fission atoms)
    - extended-defect evolution (bubbles, pores, dislocations)
    - fuel densification
    - improved model for grain growth
  - Illustration: dislocation density increases with burn-up suppressing generation of intra-granular-bubbles → stabilization of intra-granular-bubble concentration + increase in mean size + pinning of dislocations
Improvement of MFPR

- Evolution of the code to treat more than just SAs
  - Dislocation density: comparison with data from Kashibe et al. (1993)
Improvement of MFPR

- Evolution of the code to treat more than just SAs
  - Post-irradiation intra/intergranular gas distribution

<table>
<thead>
<tr>
<th>r (mm)</th>
<th>Gaz intra</th>
<th>Gaz inter</th>
<th>Rétention</th>
<th>exp</th>
<th>MFPR</th>
<th>exp</th>
<th>MFPR</th>
<th>exp</th>
<th>MFPR</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.9</td>
<td>73</td>
<td>83.8</td>
<td>14</td>
<td>6.8</td>
<td>87</td>
<td>90.6</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1.3</td>
<td>73</td>
<td>84.2</td>
<td>14</td>
<td>7.0</td>
<td>87</td>
<td>91.2</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>(79.9)</td>
<td></td>
<td></td>
<td></td>
<td>(86.6)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2.0</td>
<td>73</td>
<td>84.6</td>
<td>14</td>
<td>7.6</td>
<td>87</td>
<td>92.2</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2.4</td>
<td>87</td>
<td>84.7</td>
<td>8</td>
<td>8.2</td>
<td>95</td>
<td>92.9</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3.0</td>
<td>87</td>
<td>84.6</td>
<td>8</td>
<td>9.0</td>
<td>95</td>
<td>93.6</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>(79.3)</td>
<td></td>
<td></td>
<td></td>
<td>(88.4)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3.7</td>
<td>88</td>
<td>83.8</td>
<td>8</td>
<td>9.5</td>
<td>96</td>
<td>93.3</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Data from ADAGIO test 1065, burn-up of 60GWD/tU; Thermal & fission conditions from TOSUREP
Improvement of MFPR

- Evolution of the code to treat more than just SAs
  - DB LOCA: comparison with data from GASPARD test A₀, burn-up of 60GWd/tU

Measured Xe release:
- 5.9% during irradiation;
- 15.3% during transient
Conclusions

• Two codes are developed with different objectives
  o ASTEC/ELSA: semi-empirical for reliable and rapid calculation of release of all FPs, actinides and structural materials from degrading cores, all core configurations
  o MFPR: highly-mechanistic for insight into the state of the fuel and FPs for all types of transient, SA or otherwise

• Priorities for improvement were identified and have been partly accomplished
Conclusions

Next steps

**ELSA**: improve coverage of all releases
- Structural: must still add release of chromium, iron, niobium, nickel and zirconium
- Further improvement of Ag-In-Cd: necessary w.r.t. In.

**MFPR**: more reliable tool for analysing diverse situations (irradiation regime, transients, DB LOCA, SA)
- Fission gases: improvement of dislocation model, intergranular behaviour, key parameters...
- Chemically-active elements: thermodynamic data, diffusion coefficients, conditions of formation and behaviour of separate phases
- Extend modelling to MOX fuel and special features (e.g., rim)
- Implement code in a more global tool by coupling to a fuel code (esp. mechanical phenomena including the cladding)
Acknowledgements

- The authors thank their IBRAE colleagues, especially Drs. Berdyshev, Ozrin, Shestak, Tarasov & Veshchunov, for their theoretical insights and numerical exploits embodied in the MFPR code. The authors also thank Dr. Nicaise (IRSN) for useful ideas with respect to modelling molybdenum and barium release.

- The GASPARD and ADAGIO experiments were conducted by the Commissariat à l’Energie Atomique (CEA, France).

- This work is mainly funded via the annual grant to IRSN from the French Ministry for Ecology and Sustainable Development. Some work on ELSA has been funded by contracts with the Commission of the European Communities DGXII and on MFPR via funding from the Russian Academy of Science.