The European Commission’s science and knowledge service
Joint Research Centre

The chemistry of the MSR fuel

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Joint Research Centre and MSR activities

- Institutional projects with direct funding
  - GenIV policy support
  - Member states support
- Participation in EU HORIZON2020 project (indirect funds)
  - SAMOFAR project (2015-2019)
- Collaboration agreements with Member States
  - Netherlands – TUD, NRG (SALIEN01 irradiation - ~3M€)
  - Italy, Czech Rep., France, Slovakia
- Collaboration agreements with International partners
  - US (I-NERI)
  - China (SINAP) – general PUNE agreement
- Collaborations with start-ups (contractual work)
MSR activities at JRC

- Synthesis of An-fluoride and chloride salts
- Pyrochemical reprocessing of the fuel
- Physico-chemical properties investigation (Fuel + FP chemistry)
- Thermodynamic Database of F\(^-\) and Cl\(^-\) salts
- Irradiation & PIE of fuels
Ultimate goal of the JRC labs

• To provide experimental validation of fuel performance
• To better understand fission product chemistry
• To find a way to control redox potential of the fuel salt
• To find the best way for clean-up scheme
Challenges for experimental studies

✓ Purity of the materials
✓ How to contain the liquid?
✓ How to avoid corrosion?
✓ How to avoid vaporisation?

• Treatment with HF(g)

• Ni-based or BN container materials
• Encapsulation
Synthesis & Purification of AnF_x

- HF gas line + Inconel fluorination reactor (up to 1200° C)

- ThF₄, UF₄ and PuF₃ synthesised from low fired ThO₂, UO₂ and PuO₂ with very high purity

  \[
  \text{UO}_2 + 4\text{HF}(g) \rightarrow \text{UF}_4 + 2\text{H}_2\text{O}(g) \\
  \text{PuO}_2 + 4\text{HF}(g) \rightarrow \text{PuF}_4 + 2\text{H}_2\text{O}(g) \\
  \text{PuF}_4 + 0.5\text{H}_2 \rightarrow \text{PuF}_3 + 2\text{HF}
  \]
Purity check

weight balance check
m (UO₂) vs. m (UF₄)

color check

Melting point determination

XRD phase analysis
Salient irradiation experiment in HFR-Petten

Goal: Fission product behaviour in salt, graphite and metallic specimens

- $\text{ThF}_4$-LiF eutectic mixture

- Corrosion-resistant graphite crucible
- Open container (metallic filter) to accommodate FG release
- Crucible wall temperature maintained at $T_{\text{melt}} + 50$ K
- Neutron fluence monitored through activation sets
The experimental approach for phase diagram studies
Phase diagram study of the LiF-PuF$_3$ system
Method to measure enthalpy of mixing
Enthalpy of mixing of the LiF–KF system. (●) This study at T = 1121 K. (▲▼) Hong and Kleppa at T = 1176 K and T = 1360 K.

Enthalpy of mixing of the LiF–ThF$_4$ system. (○, ●) This study at T = 1121 K and T = 1383 K. Solid line: Calculated enthalpy of mixing from the assessment. Dashed line: Calculated enthalpy of mixing from earlier assessment.
LiF-ThF₄ phase diagram revisited

Left graph: Comparison between the LiF vapour pressure (monomer) for the pure LiF liquid phase and for the LiₓTh₁₋ₓF₄₋₃ₓ liquid solution.

Right graph: Comparison between the ThF₄ vapour pressure for the pure ThF₄ liquid phase and for the LiₓTh₁₋ₓF₄₋₃ₓ liquid solution.

The vapour pressure of ThF₄ has been extrapolated for temperature lower than the melting point from the equation of the liquid state.
LiF – ThF₄
Vapour pressure - Knudsen cell MS

- to demonstrate retention of FP in the fuel matrix
- to determine volatility of the fuel
- to determine thermodynamic stability
- to determine gas composition

CsF is one of the stable form of Cs-FP in the MSR fuel:

\[ \Delta G(F_2) \sim MSFR, T=900K \]

\[ Cs \rightarrow \text{CsF} \]
Heat capacity determination of ThF$_4$ containing salts

- Heat capacity of ThF$_4$ and selected LiF–ThF$_4$ compositions measured (method improved and optimized)
Thermal conductivity

Laser flash technique

New crucible designs made to optimise the data output
Conclusions

We master:
- synthesis of An fluorides
- electrochemical studies
- melting points (FP effect)
- phase diagrams (exp. + modelling) (FP effect)
- vapour pressures (FP effect)
- heat capacity
- mixing enthalpy
- FP release from fuel (PIE capacity included)

Under development:
- Raman studies – structure
- Thermal conductivity (Phd on it)
- Viscosity (Phd on it)
- Density (Phd on it)

We own:
- JRCMSD Salt Database
  share through TAF-ID project
Conclusions

- Still gaps on physico-chemical data of MSR fuels

- Physico-chemical models are under development, and experimental validation is essential

- JRC has developed unique techniques and methods for An-chemistry in molten salt