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WP3: Source term distribution and mobility

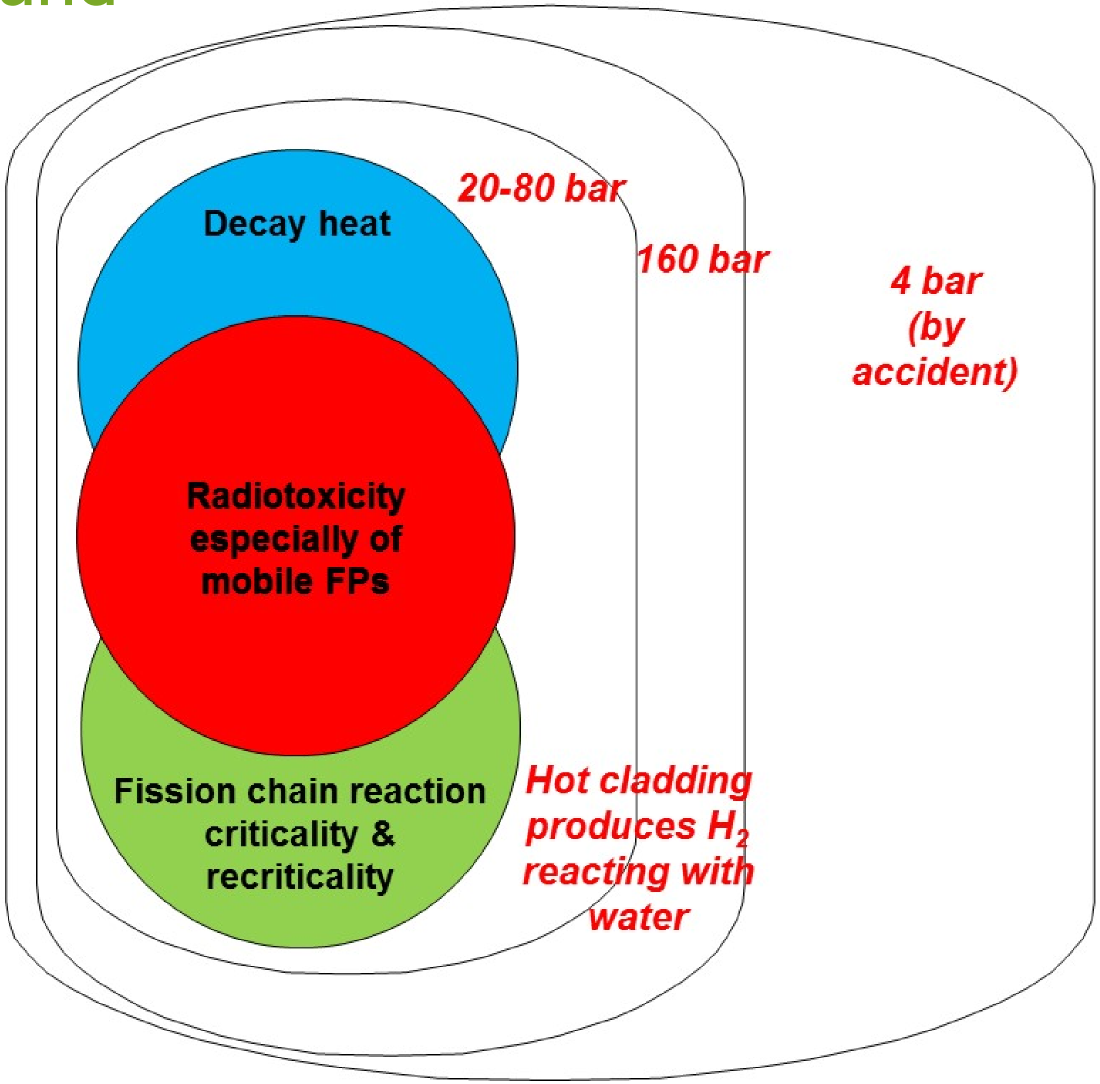
Final Meeting

28 November 2023, Avignon

WP3: Scientific background

- **NRC source term definition:**
  Types and amounts of radioactive or hazardous material released to the environment following an accident.
- Its **complex assessment** is based on:
  - Radioactive material **composition**
  - Its chemical **mobility** / activity
  - Presence of **driving forces**
  - Presence of **barriers**
- Safety of **existing LWR** is high; nonetheless, based on substantial **driving forces, mechanical barriers***, and their **complex protection** system.

  * *filtered venting is the only non-mechanical barrier*



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WP3: Scientific background

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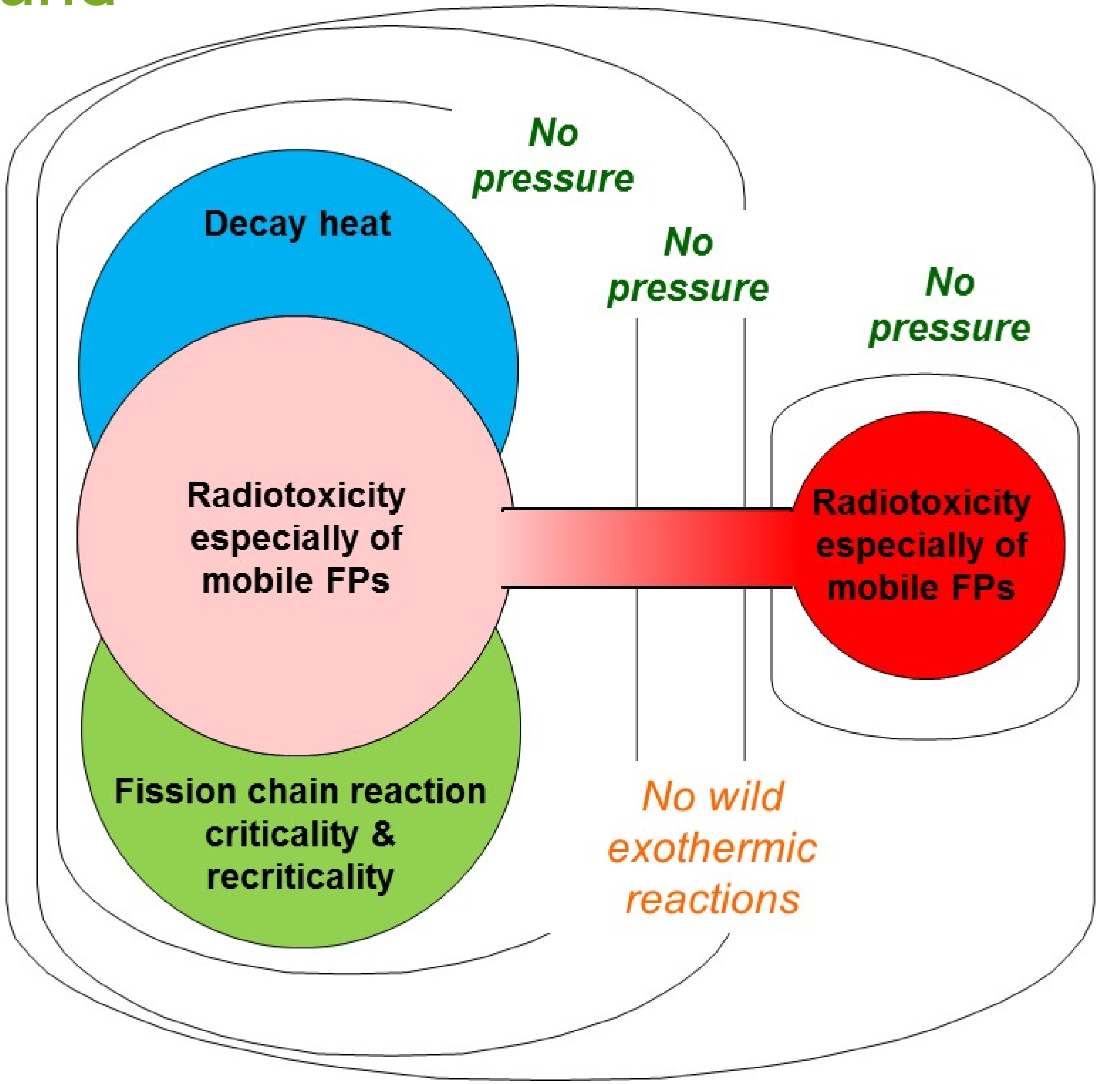
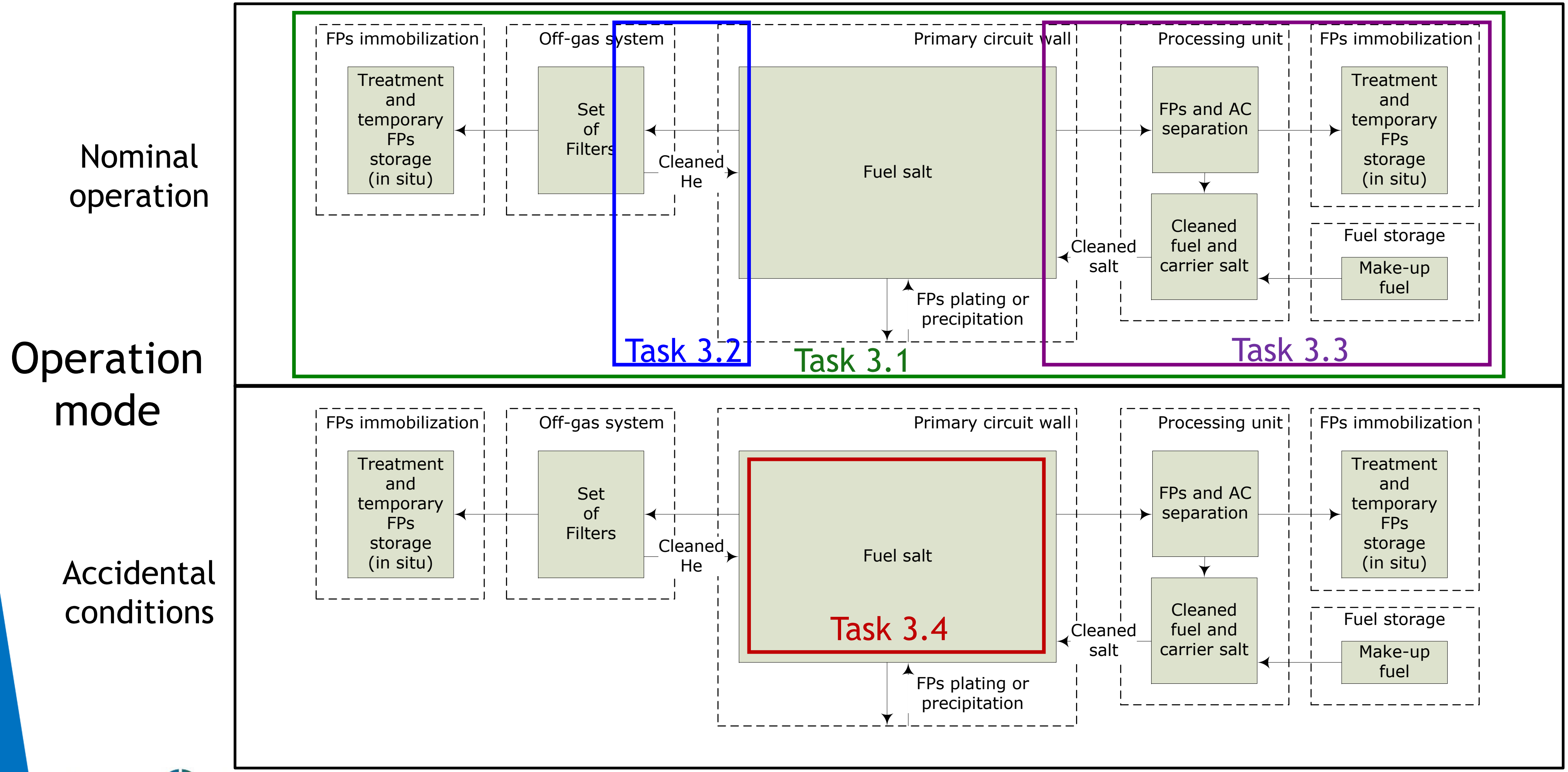
- Its **complex assessment** is based on:
  - Radioactive material **composition**
  - Its chemical **mobility** / activity
  - Presence of **driving forces**
  - Presence of **barriers**
- **MSR with liquid fuel** is special:
  - Chemical mobility can be controlled.
  - Driving forces can be avoided.
  - Mechanical barriers “robustness” can be reduced.
  - Barriers can/should be also chemical.
  - Safety philosophy can be oriented towards control of the fuel state (temperature, location, redox pot.) rather than on barriers protection.

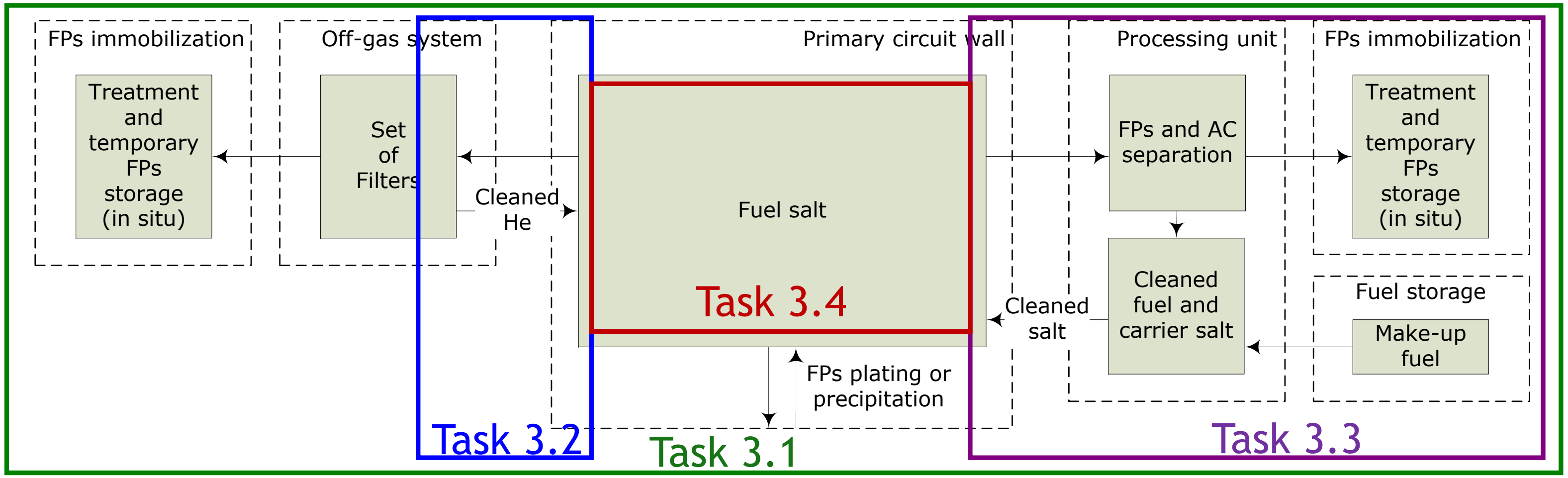


WP3: Tasks and source term locations



WP3: What is not addressed

- Mechanical and chemical barriers
  (except for aerosol filters and removed FPs immobilization).
- Chemical and mechanical stability of barriers
  (e.g. vessel disintegration).
- Source term mobility at accidental conditions in FPU and off-gas system.
- Presence of driving forces: exothermic reactions within salt, metals, concrete, water, etc.
  (except of expert judgements / literature survey, especially for fluoride volatilization process).



WP3: Tasks and internal and external dependency

- **Task 3.1 Source term distribution** (M01 – M48); **CNRS**, PSI, POLIMI
  - → Material exchange coefficients at interfaces from Task **3.2** and **3.3**
  - ← Actinides and fission product composition provided to **WP1,2 & 4** and Tasks **3.2**, **3.3**, **3.4**
- **Task 3.2 Removal rates to the off-gas system** (M01 – M48); **NRG**, TU Delft, POLIMI
  - → Actinides and fission product composition provided from Task **3.1**
  - ← Material exchange coefficients at interfaces to Tasks **3.1**
- **Task 3.3 Source term in the reprocessing and storage** (M01 – M48); **CNRS**, JRC, CEA, CV REZ
  - → Actinides and fission product composition provided from Task **3.1**
  - ← Material exchange coefficients at interfaces to Tasks **3.1**
  - ← Fuel processing unit design to **WP1**
- **Task 3.4 Source term in the core** (M01 – M48); **PSI**
  - → Actinides and fission product composition provided from Task **3.1**
  - ← Source term release from the fuel salt to containment and filtering options to **WP1,4 & 6**

WP3: Deliverables & Milestones

Deliverables

- D3.1: Distribution of fission products in the representative MSR system (M48 – CNRS) *Delivered*
- D3.2: Material exchange on the interface between salt and off-gas systems (M48 – NRG) *Delivered*
- D3.3: Material exchange with the reprocessing unit (M48 – CNRS) *Delivered*
- D3.4: Immobilization of the fission products from reprocessing unit (M48 – CNRS) *Delivered*
- D3.5: Aerosols formation and filtration in accidental conditions (M48 – PSI) *Delivered*
- D3.6: Burnup tools verification by incremental benchmark (M48 – PSI) *To be submitted in few days*

Milestones

- MS5 – Technical note (M6-CNRS):
  Initial distribution of FPs and the reprocessing scheme *Delivered*
- MS8 – Draft of D3.2 (M36-NRG): *Delivered*
  Updated removal rates to off-gas system
- MS6 – Draft of D3.3 (M36-CNRS): *Delivered*
  Updated removal rates and residence times in Fuel Reprocessing Unit (**FPU**)
- MS7 – Draft of D3.1 (M40-CNRS): *Delivered*
  Updated distribution of fission products

Task 3.2: Removal rates to the off-gas system

Stefano Lorenzi (POLIMI) and Edo Frederix (NRG)

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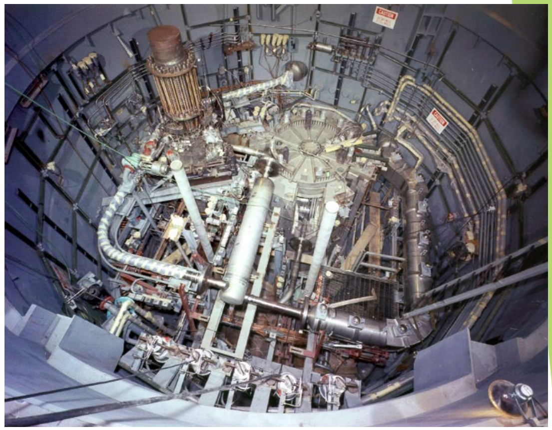
Lessons learned from the MSRE on fission product removal



- Molten Salt Reactor Experiment at Oak Ridge in the 60s
- Three groups of fission products:
  - Salt seekers
  - Noble gases (Xe, Kr) → neutron poison
  - Noble metals (Nb, Mo, Tc, Ru, Ag, Sb, Te) → decay heat. E.g., from E.L. Compere[1]:

  *"They provide **fixed sources of decay heat and radiation**. The afterheat effect will require careful consideration in design, and the associated radiation will make maintenance of related equipment more hazardous or difficult."*

- Idea to remove noble gases and noble metals by bubbles:
  - From R.J. Kedl[2]: *"These bubbles manifested themselves in several ways in the operation of the MSRE. In one sense their presence was unfortunate because it complicated the understanding of many observations in the reactor, but in another sense **it was fortunate because it led to the suggestion of efficient ways of removing fission products** (particularly noble gases, but possibly also noble metals) from future molten-salt reactor systems."*
  - From R.J. Kedl and A. Houtzeel[3]: *"**The circulating helium bubble concept should be considered seriously as a ^{135}Xe removal mechanism in future molten-salt reactors**. Helium bubbles could be injected into the flowing salt at the core outlet and be removed with an in-line gas separator some distance downstream."*

[1]E.L. Compere, S.S. Kirslis, E.G. Bohlmann, F.F. Blankenship, and W.R. Grimes. Fission product behavior in the molten salt reactor experiment. Technical report, Oak Ridge National Lab.(ORNL), Oak Ridge, TN (United States), 1975.
[2]R.J. Kedl. Migration of a class of fission products (noble metals) in the molten-salt reactor experiment. Technical report, Oak Ridge National Lab., Tenn.(USA), 1972.
[3]R.J. Kedl and A. Houtzeel. Development of a model for computing 135Xe migration in the MSRE. Technical report, Oak Ridge National Lab., 1971.

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Task 3.2: Removal rates to the off-gas system

- How fast are Gaseous Fission Products (GFPs) and Solid Fission Products (SFPs) removed? From S. Delpech et al.:

  *First, an on-line gaseous extraction with helium bubbling removes all gaseous fission products and noble metals. In our simulations, **the extraction time of these elements is assumed to be 30 s**.*

- Can we model this?
  - POLIMI: GFPs
  - NRG: SFPs

[1]S. Delpech, E. Merle-Lucotte, D. Heuer, M. Allibert, V. Ghetta, C. Le-Brun, X. Doligez, and G. Picard. Reactor physic and reprocessing scheme for innovative molten salt reactor system. Journal of fluorine chemistry, 130(1):11–17, 2009.

Gaseous fission products: Modelling approach

- **Starting point:** multiphysics tool in OpenFOAM (neutronics + thermalhydraulics). Solver for two compressible phases, adopting a Eulerian-Eulerian approach
- **New capability**: Multicomponent modelling for the GFPs: production, consumption, transport and exchange of GFPs in the liquid-salt and gaseous-helium phases

$$liquid\ phase: \frac{\partial \alpha_l \rho_l Y_{Xe,l}}{\partial t} + \nabla \cdot (\alpha_l \rho_l \mathbf{u}_l Y_{Xe,l}) - \nabla \frac{\alpha_l \mu_l}{\mathrm{Sc}_l} \nabla (Y_{Xe,l}) = \frac{dm_{Xe,l}}{dt} + P + C_l$$

$$gaseous\ phase: \frac{\partial \alpha_g \rho_g Y_{Xe,g}}{\partial t} + \nabla \cdot (\alpha_g \rho_g \mathbf{u}_g Y_{Xe,g}) - \nabla \frac{\alpha_g \mu_g}{\mathrm{Sc}_g} \nabla (Y_{Xe,g}) = \frac{dm_{Xe,g}}{dt} + C_g$$

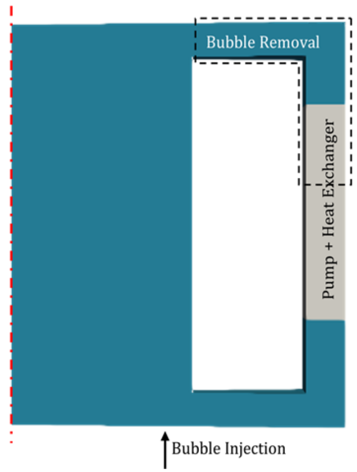
$$\frac{dm_{Xe,k}}{dt} = \rho_k K_{Xe,k} a_k (Y^*_{Xe,k} - Y_{Xe,k}) \qquad P = \Sigma_f \phi \cdot y_{Xe} \cdot (m_{mol}/N_{Av}) \qquad C_k = -\alpha_k \rho_k (\lambda_{Xe} + \sigma_a \phi) Y_{Xe,k}$$

- For the mass transfer term, Henry's law for interfacial composition and Higbie correlation for Sherwood number for mass transfer coefficient

$$Y^*_{i,k} = H\left(\frac{Y_{i,j}\rho_j}{\rho_k}\right) \qquad K_{i,k} = \frac{\mathrm{Sh} \cdot D_{i,k}}{d_b} \qquad \mathrm{Sh} = 1.13\ \mathrm{Re}^{1/2}\mathrm{Sc}^{1/2}$$

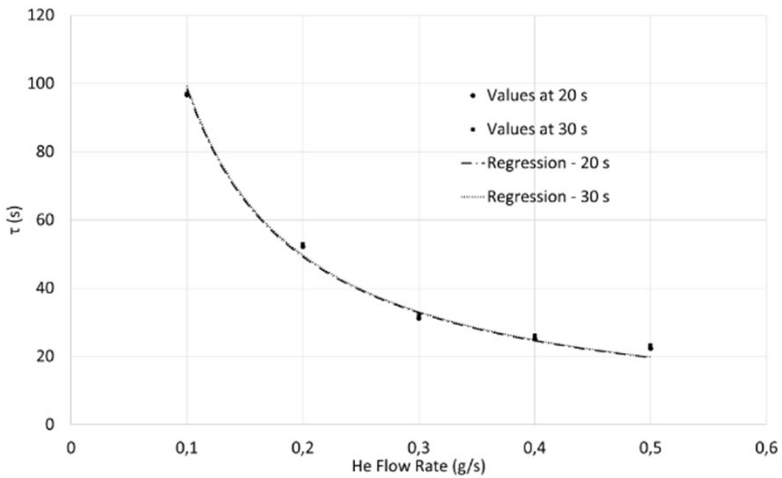
GFP: Results achieved

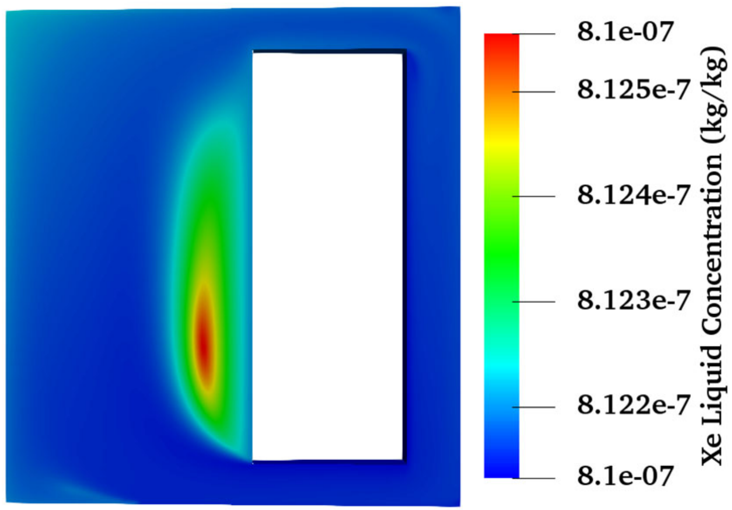
- Two geometries: squared axial-symmetric and 3D realistic geometry
- Analytical verification on 1D flow
- Cycle time calculated for axial-symmetric between 100 s and 20 s according to the helium mass flow rate injection - 0.1 to 0.5 g/s



$$\frac{\partial N}{\partial t} = (y\Sigma_f - \sigma_a N)\,\phi - \gamma_{bub} N$$

$$\frac{\dot{X}e_{outflow}\,(kg/s)}{Xe_{mass}\,(kg)} = \frac{\gamma_{bub} Xe_{mass}}{Xe_{mass}} = \gamma_{bub}\,(1/s)$$





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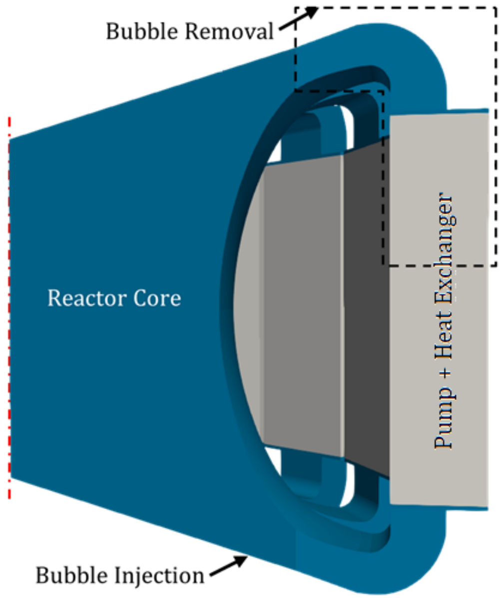
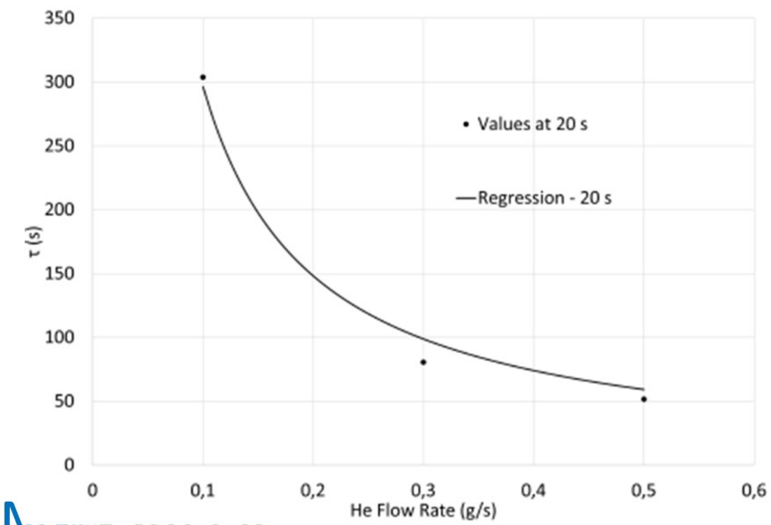
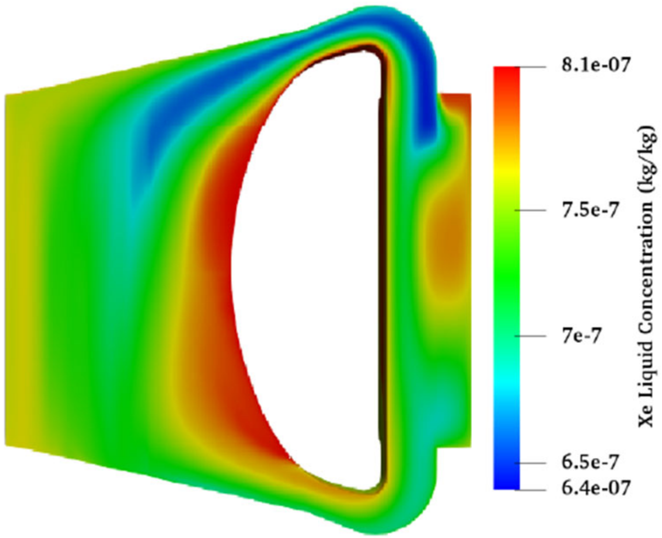
Results achieved

- 3D realistic geometry
- Cycle times calculated for 3D realistic geometry are compatible with the ones calculated for the axial symmetric geometry
  - Axial-symmetric geometry = 5°
  - 3D geometry with just Xe-135 = 90° (1/4th of the entire reactor)
  - 3D geometry with Xe-family = 22,5° (1/16th of the entire reactor)







Solid fission products

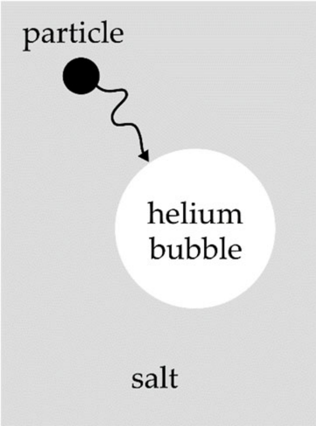
- From M.W. Rosenthal et al.[1]:

  *"…but the particles are believed to be sufficiently small for the transport to be similar to that of molecular species. On the basis of this assumption, **the mass transfer coefficients for the metal particles would be proportional to those that have already been calculated for xenon and krypton**."*

- From R.J. Kedl[2]:

  *"… some credence must be given to the hypothesis that **noble metals migrate according to the simplest form of mass transfer theory**."*

- So, fission product particles diffuse → diffusivity is **particle size dependent**
- Particle size distribution depends on balance between:
  - Production rate of noble metal atoms (fission/decay)
  - Growth of colloidal particles by coagulation
  - Removal by 'surface':
    - Bubbles: flotation → investigated in SAMOSAFER
    - Solid surfaces: plating



[1]M.W. Rosenthal, R.B. Briggs, and P.R. Kasten. Molten-salt reactor program semiannual progress report for period ending February 28, 1969. Technical report, Oak Ridge National Lab.(ORNL), Oak Ridge, TN (United States), 1969.
[2]R.J. Kedl. Migration of a class of fission products (noble metals) in the molten-salt reactor experiment. Technical report, Oak Ridge National Lab., Tenn.(USA), 1972.

Noble metal flotation model

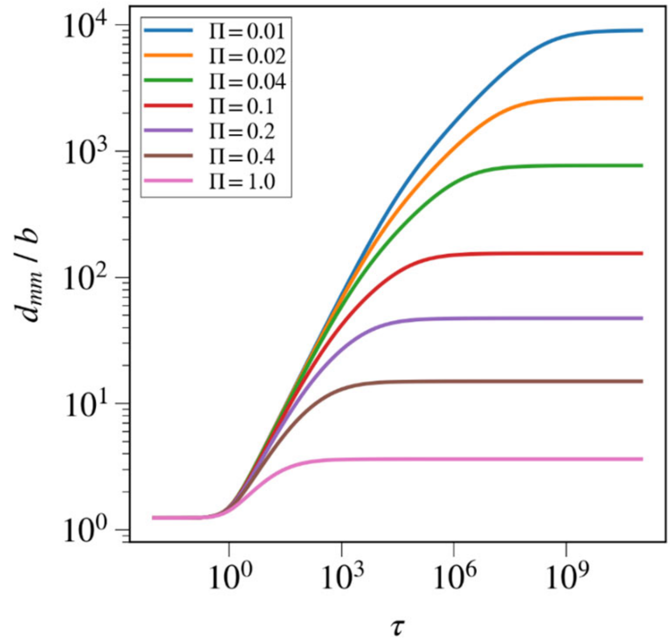
- Method of moments used to solve for the evolution of the particle population in the MSR
- Model solution is self-similar, depending on a single parameter Π:

Parameter:

$$\Pi = \frac{\lambda a_i}{b}\sqrt{\frac{K}{F}}$$

with: mass transfer coefficient λ, interfacial area a_i, noble metal atom size b, coagulation coefficient K and production rate F.

- **Knowing Π gives us the equilibrium mean particle size and removal rate!**
- **However, value of Π depends on the bubbles in the MSR → how do they behave?**



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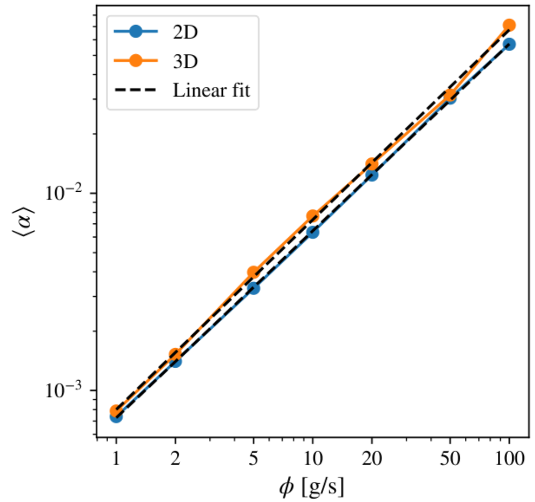
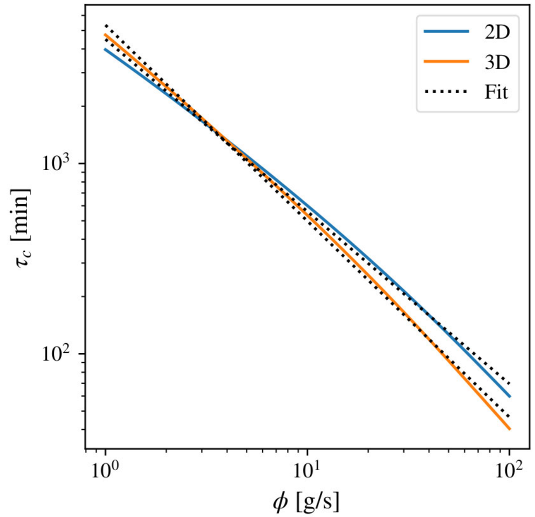
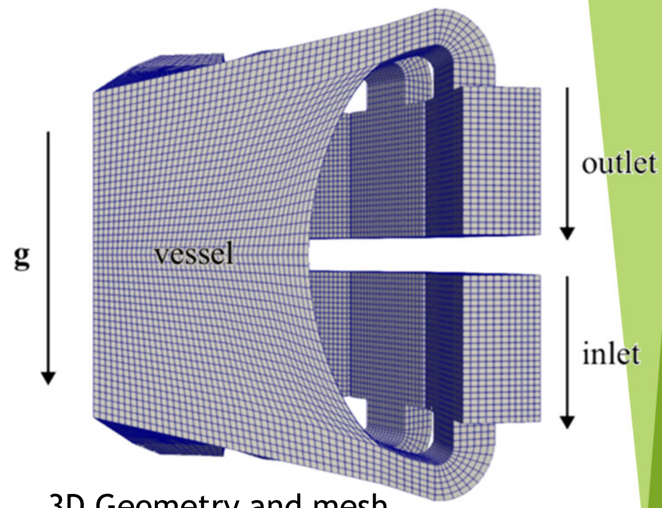
Simulation of bubbles in the MSFR

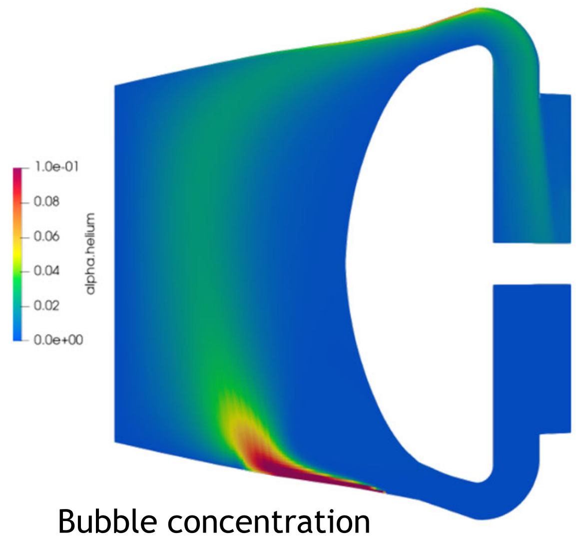
- CFD simulation of bubble injection in the MSFR
- Model that takes into consideration: turbulence, bubble breakup and coalescence, removal of bubbles near the outlet.
- Simulation produces dependence of mean bubble interfacial area on bubble injection rate → prediction of Π → prediction of removal rate







3D Geometry and mesh



Bubble concentration

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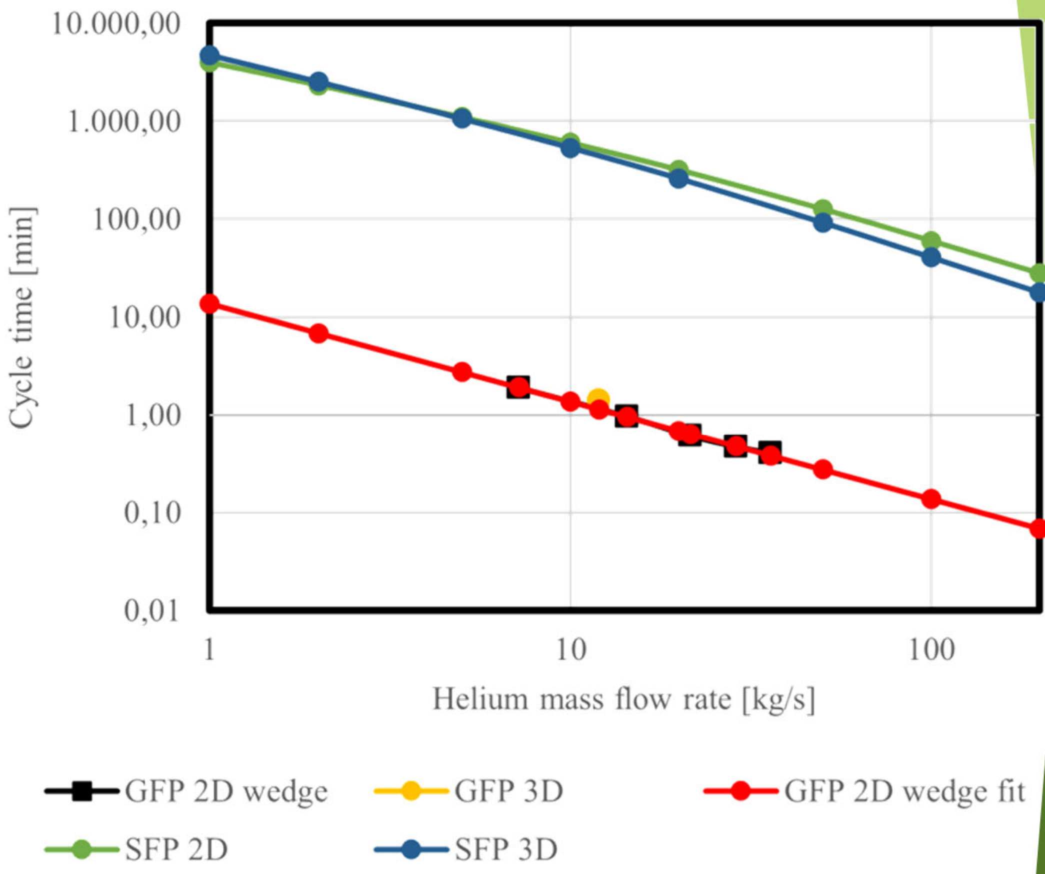
Conclusions: GFP and SFP removal rates

- GFP and SFP removal rates were calculated for several helium bubble injection rates, using CFD and theoretical modeling
- Main outcome: **improved estimates of cycle times of both GFPs and SFPs** (see figure)
- **Earlier assumption of 30 s can be reasonable for GFPs, but it orders too low for SFPs**
- However, from S. Delpech et al.[1]:

"In our simulations, the extraction time of these elements is assumed to be 30 s. As a matter of fact, lower extraction efficiency would not significantly affect the neutronic of the core. Indeed, the breeding ratio is almost unaffected if these 30 s become a few days."



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Task 3.3: Removal rates to the off-gas system

S. Delpech, P. Soucek, J. Uhlíř, M. Mareček, M. Cihlář. Serp, D. Rodrigues, C. Cannes

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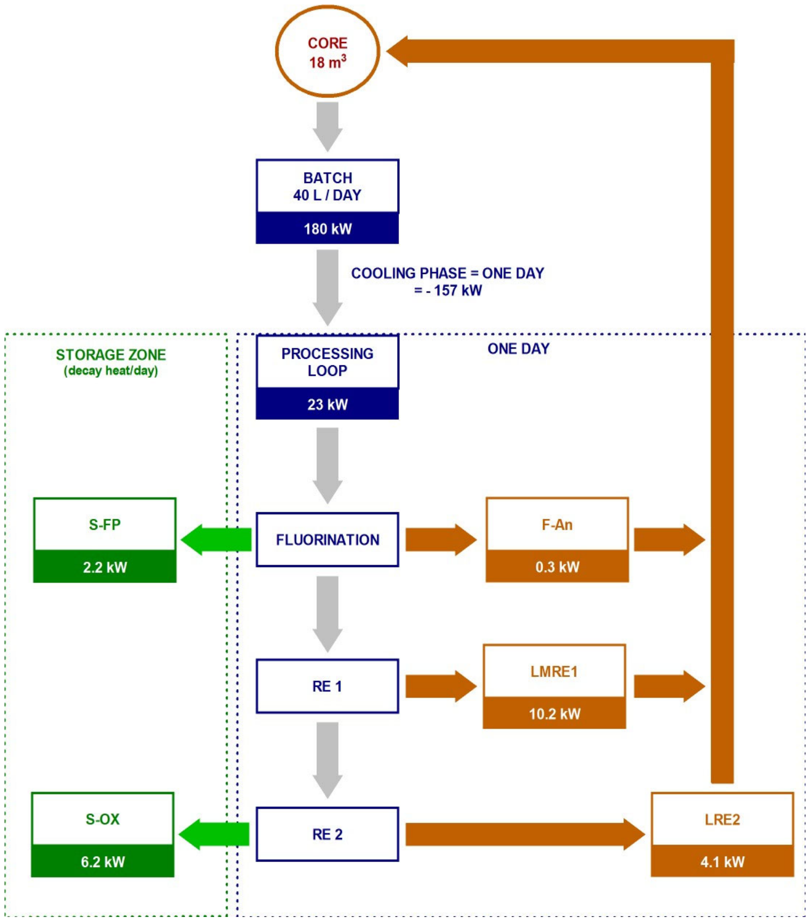
Task 3.3: Material exchange with the reprocessing unit

Distribution decay in the reprocessing plant



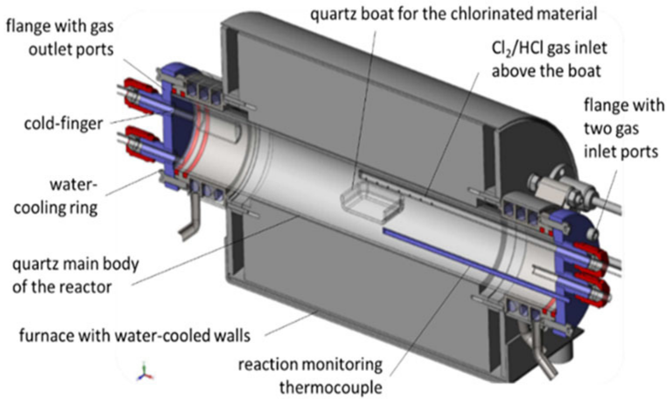
Articulation of this task around several spots

- Determination of the isotopes flux in the reprocessing plant
- Tests of reprocessing steps : fluoration, reductive extraction, precipitation
- Actinides synthesis
- Proposal of reprocessing scheme for chloride fuel salt
- Wastes management proposal

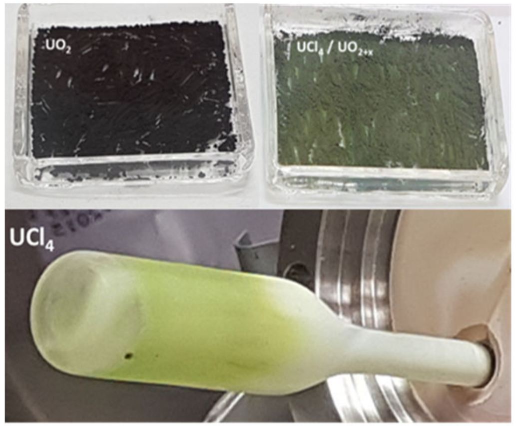
JRC | CVRez | CNRS | CEA

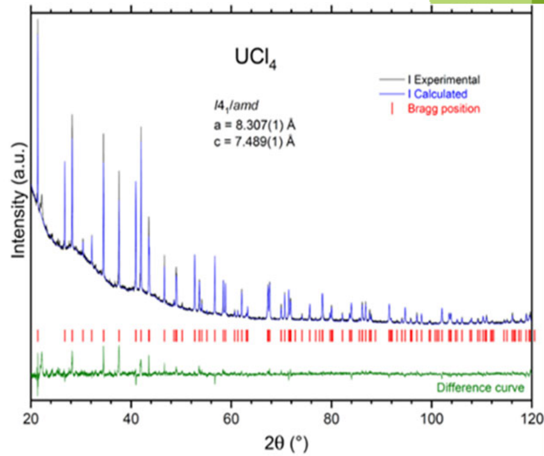
Fisrt step of experimental studies : Actinides fluoride and actinides chloride synthesis

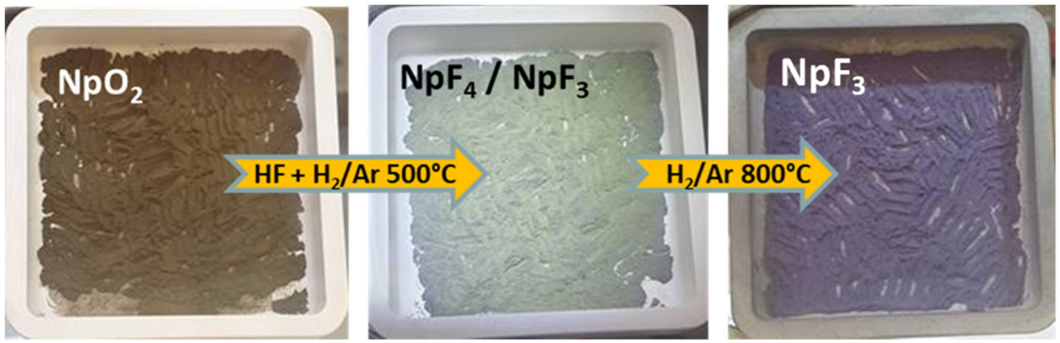
JRC

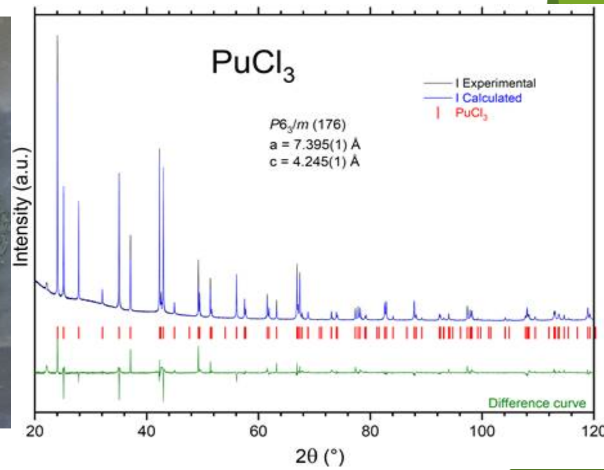


Chlorination device









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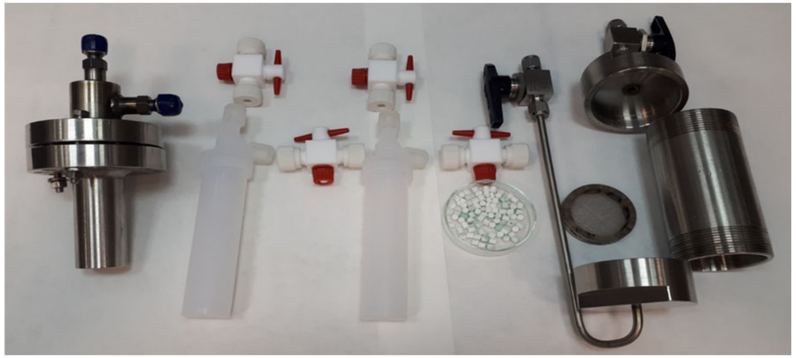
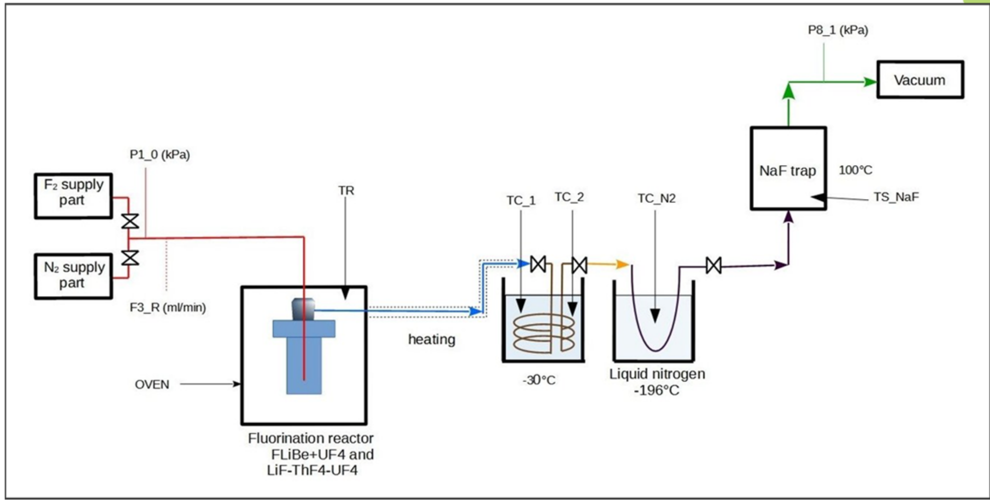
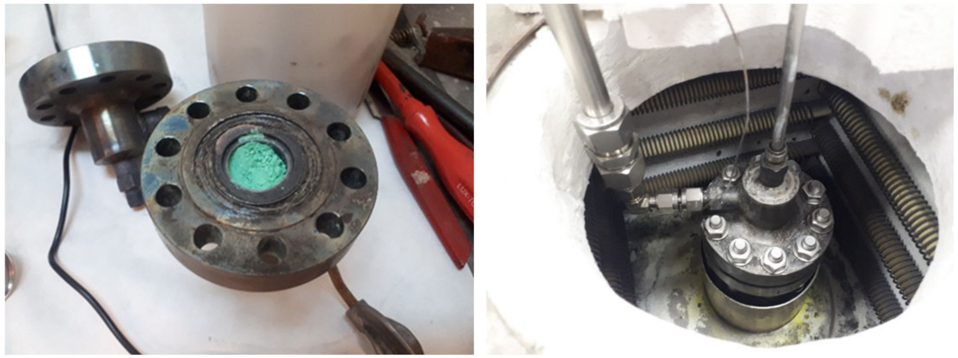
Fluorination tests

CVRez



Apparatus used for the experiment





Molten salt including UF_4 in the reactor and in the furnace

Corrosion of fluorine feed made of pure Ni tube after fluorination

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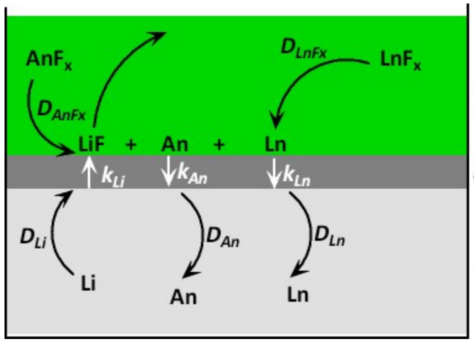
Reductive extraction

CNRS

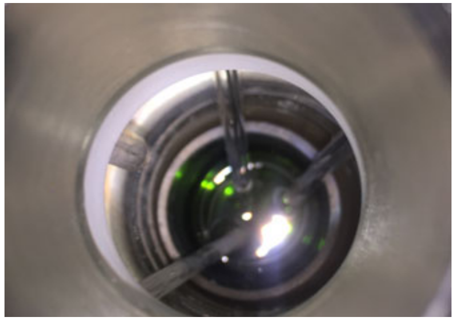


Reductive extraction principle

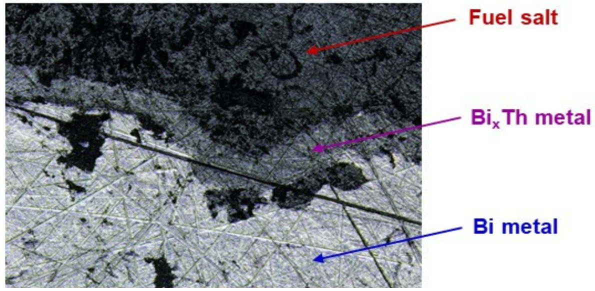
BiTh or Bi$_4$Th$_3$ produced by the chemical reactions:

$$4Li + ThF_4 + Bi \rightarrow ThBi + 4LiF$$

$$12Li + 3ThF_4 + 4Bi \rightarrow Th_3Bi_4 + 12LiF$$



FLiNaK molten salt containing UF$_4$



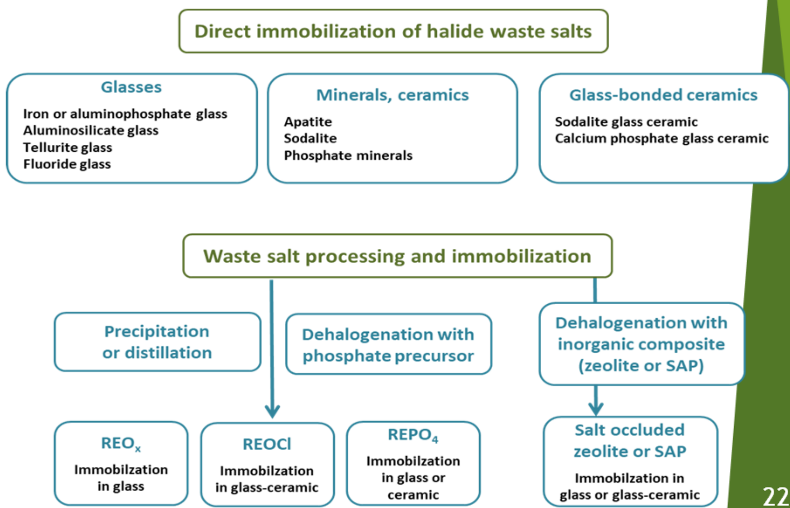
Cross section of Bi/salt interface after reductive extraction in LiF-ThF$_4$

Low efficiency of U extraction on Bi
Electrolysis limited by Na reduction?

Molten salt	I (A) set	Q (C)	ICP-OES measurements			
			n Li (mol)	n K (mol)	n Na (mol)	n Nd or U (mol)
LiF-NaF-KF + NdF$_3$ 0.17 mol%	-0.3	700	> 1.0E-07	3.15E-03	2.37E-04	2.58E-06
LiF-NaF-KF + UF$_4$ 0,22 mol%	-0.3	690	> 1.0E-07	2.91E-03	1.80E-04	> 1.0E-07

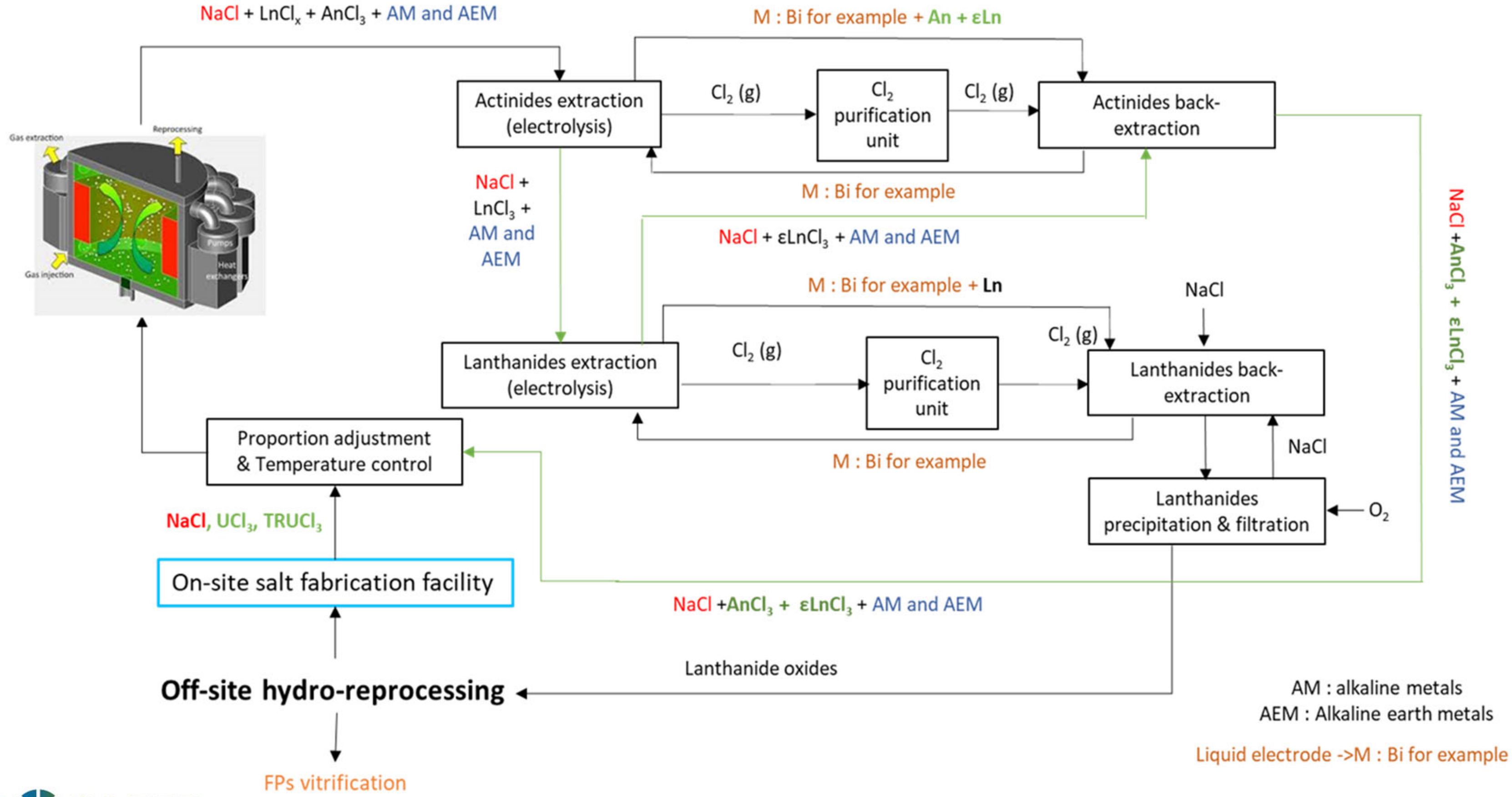
Waste management routes

CNRS



CEA-CNRS

Fuel reprocessing scheme for chloride MRS concept



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Task 3.4: Source term in the core

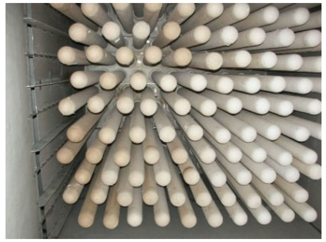
Jarmo Kalilainen (PSI), Sergii Nichenko (PSI), Jonathan Dietz (PSI), Terttaliisa Lind (PSI)

SAMOSAFER Final Meeting

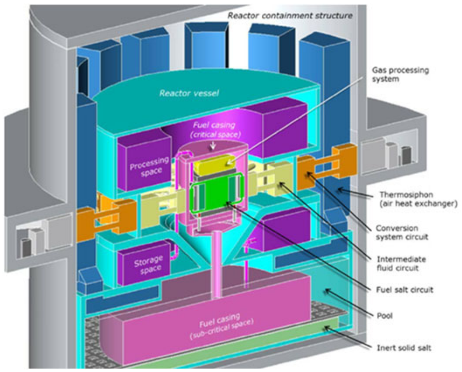
28 November 2023, Avignon, France

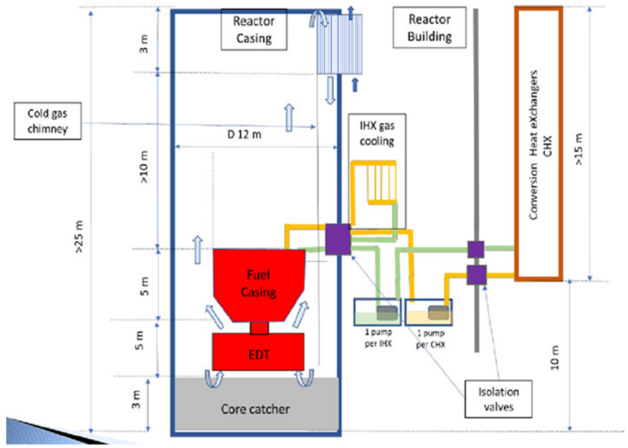
Task 3.4: simulation of severe accident in MSFR

- The simulated scenario assumes salt spill at the bottom of the containment.
- The results are published in deliverable
  D3.5: Aerosols formation and filtration in accidental conditions
- and also in
  - *Nichenko, Sergii , Jarmo Kalilainen and Terttaliisa Lind, 'MSR simulation with cGEMS: Fission product release and aerosol formation', J. Nucl. Eng. 2022, 3(1).*
  - *Kalilainen, Jarmo, Sergii Nichenko, Jiri Krepel, 'Evaporation of materials from the molten salt reactor fuel under elevated temperatures', Journal of Nuclear Materials 533 (2020).*
  - *Kalilainen, Jarmo, Sergii Nichenko, Jiri Krepel, MSR simulations with cGEMS, to be presented at the 2021 VIRTUAL CSARP Meeting, June 7-11, 2021*

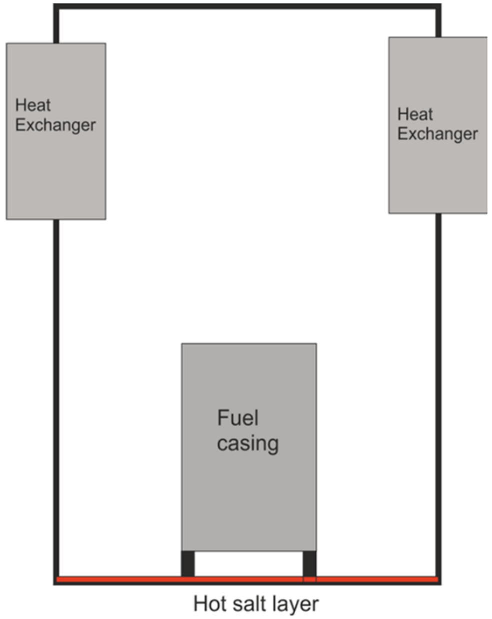


Flue gas filter for T = 250-100 °C Rath-Group, 2019 https://www.rath-group.com/en/



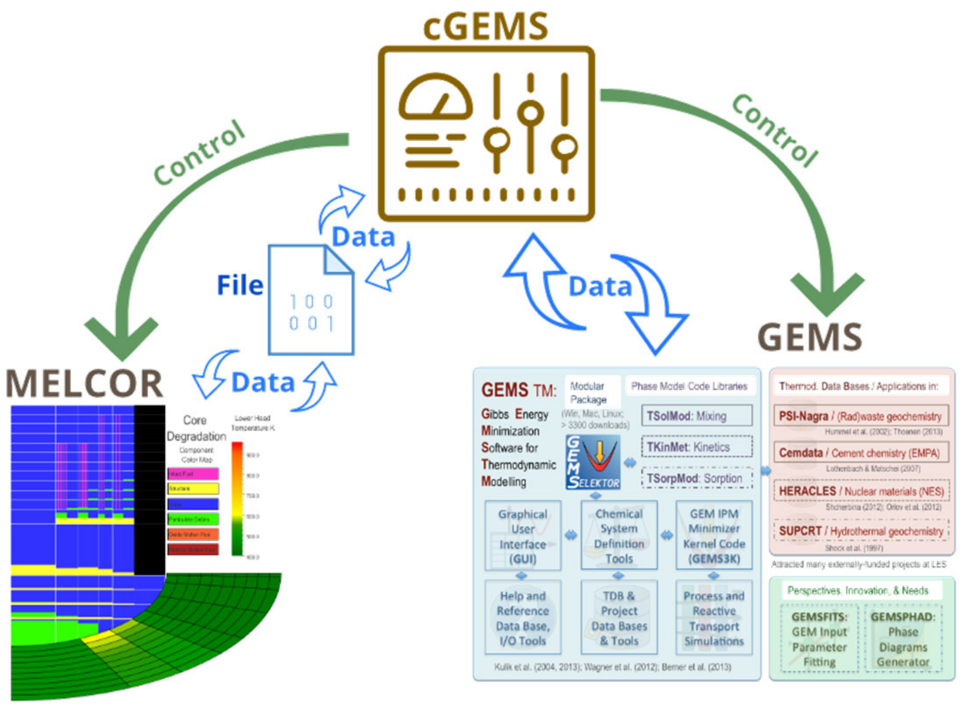


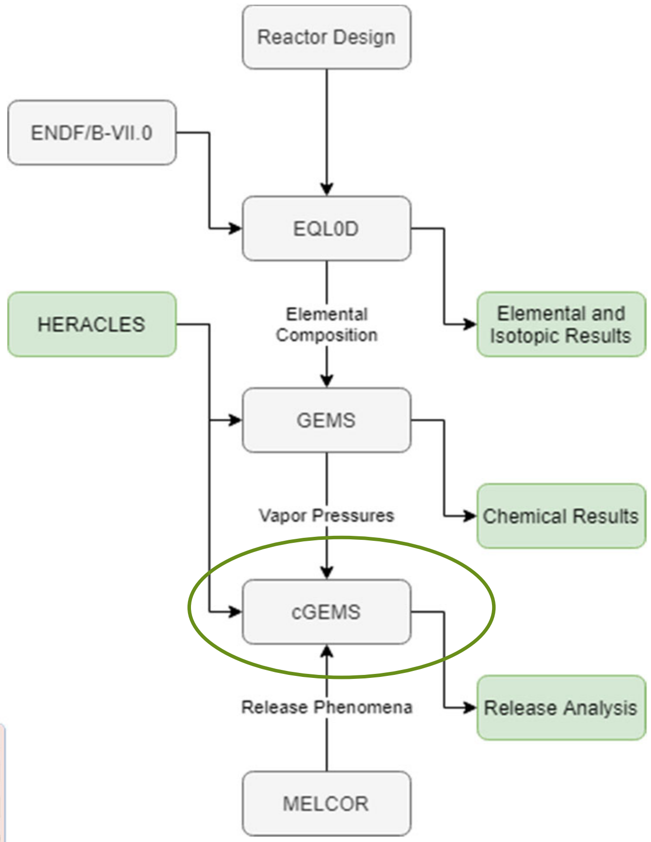
From the SAMOFAR Final meeting, E. Merle et al.



Task 3.4: cGEMS code

- cGEMS code characteristics:
  - Composition of the salt from the EQL0D simulations
  - Uses the updated HERACLES database in GEMS software
  - Li, F, U, Th, Cs, Ba, Pu, Sr, La, Zr, Ce, Np, Nd extended system
  - The data exchange between MELCOR and GEMS: cGEMS





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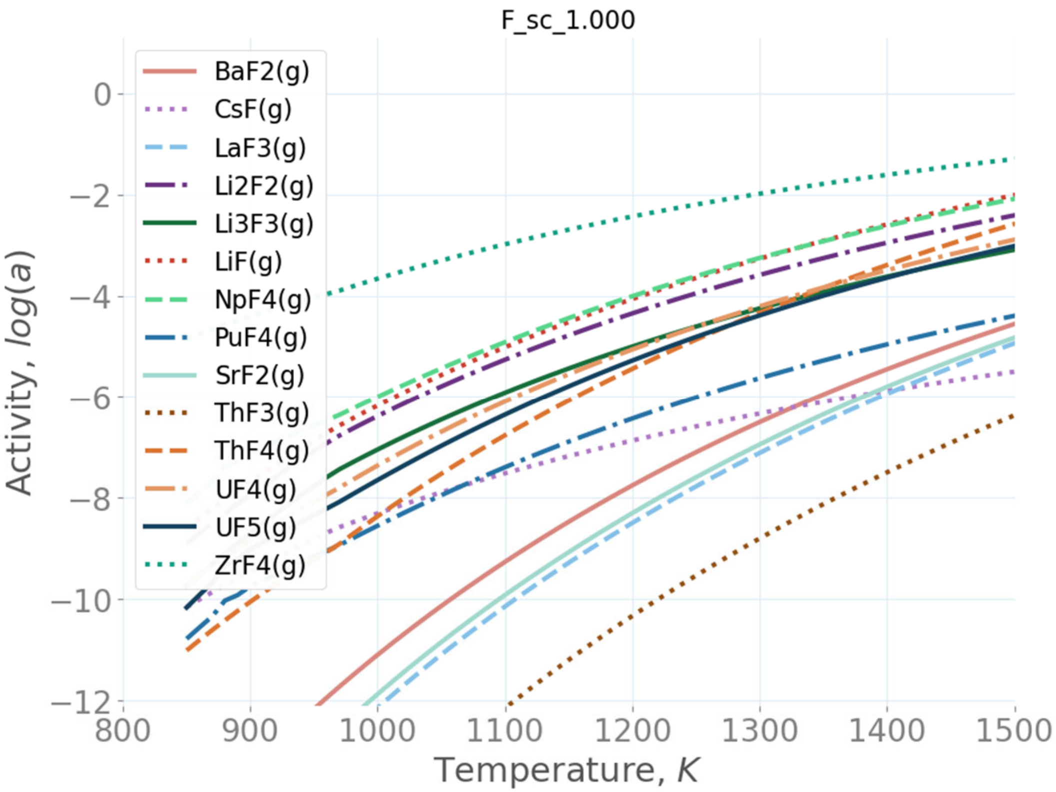
Task 3.4: activity obtained by GEMS

- For the Task3.4 Heracles database of the GEMs code was extended.

Species	Changes Made
$ThCl_4$	Imported as is from literature
Np	Imported as is from literature
$PuCl_3$	Adjusted previously existing data entry to conform with literature melting point
UCl_3	Missing liquid phase data manually matched based on literature values
NpF_3	Missing liquid phase constructed from melting-/boiling points and similarity to UF_3
AmF_3	Solid adjusted and liquid designed from assumed similarity to UF_3
ZrF_4	Imported as is from literature
$NdCl_3$	Imported as is from literature
$PrCl_3$	Imported as is from literature
PrF_3	Imported as is from literature
Na_2ThCl_6	Created in GEMS function ReacDC
Pr	Imported as is from literature

Additional Changes were made to:
NPF_4, NdF_3, SrF_2, LaF_3, CeF_3, BaF_2, CsF

- GEMS code was applied to obtain the vapor pressures.



Compounds activity (proportional to vapor pressure) as a function of temperature

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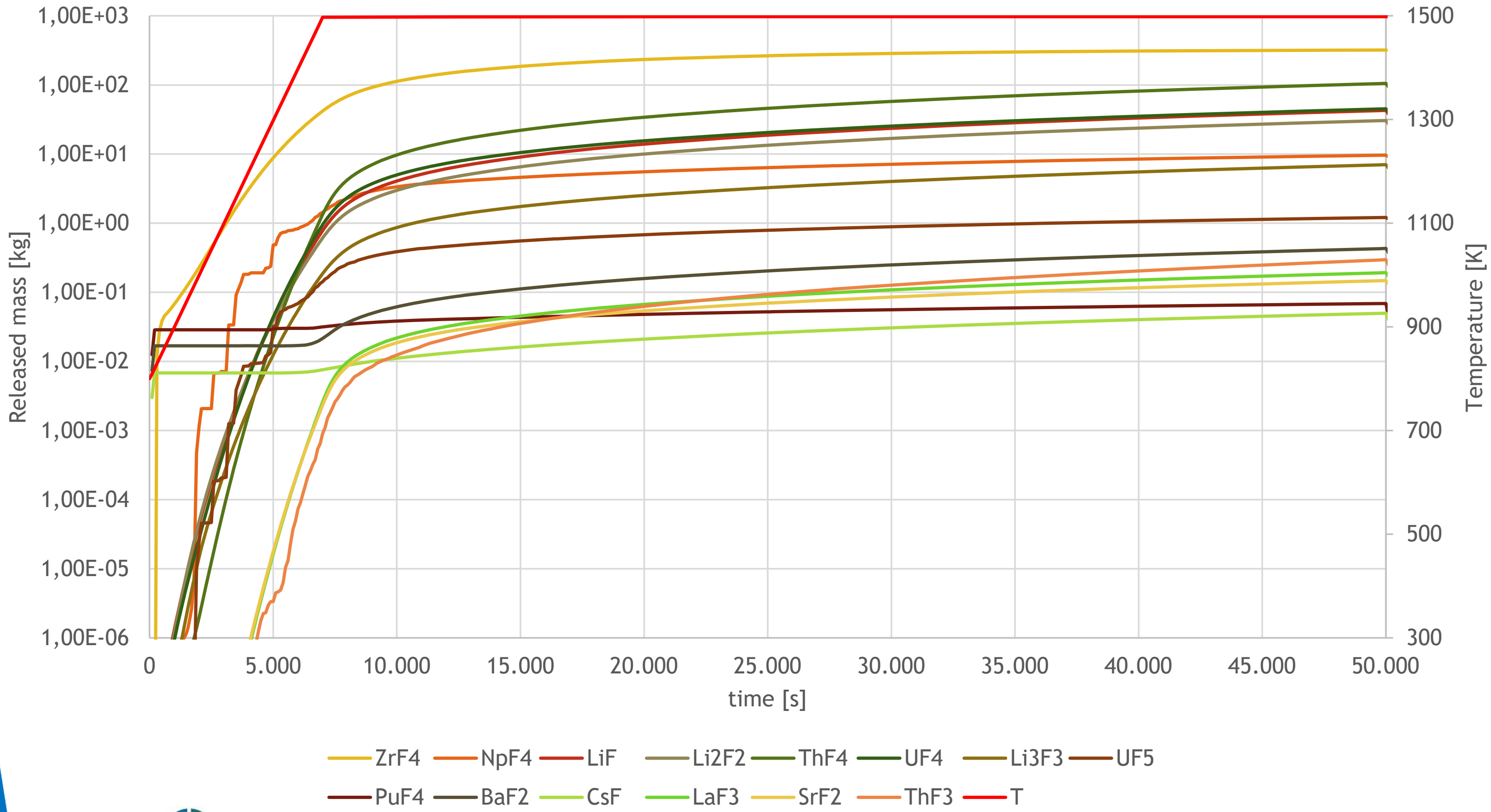
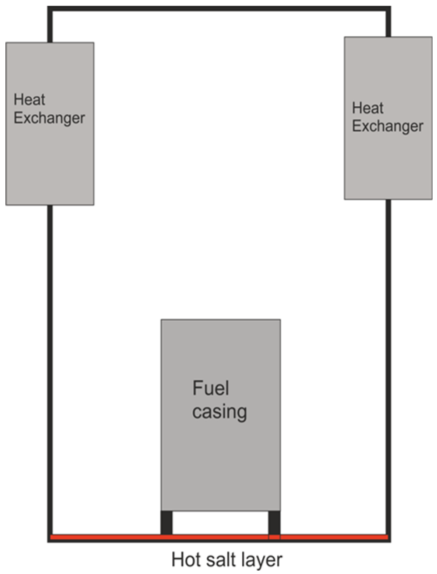
Task 3.4: released mass (cGEMS simulation)

- The coupled code was applied to simulate the release of compound from the spilled salt.

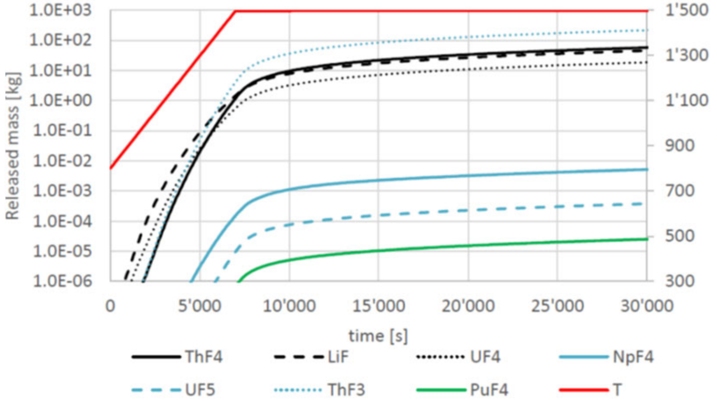


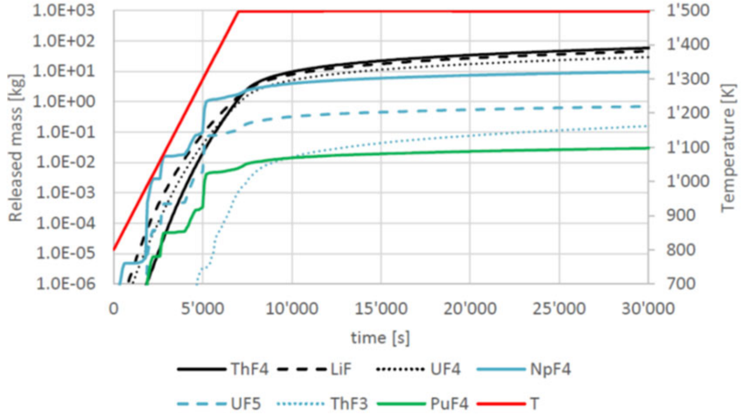


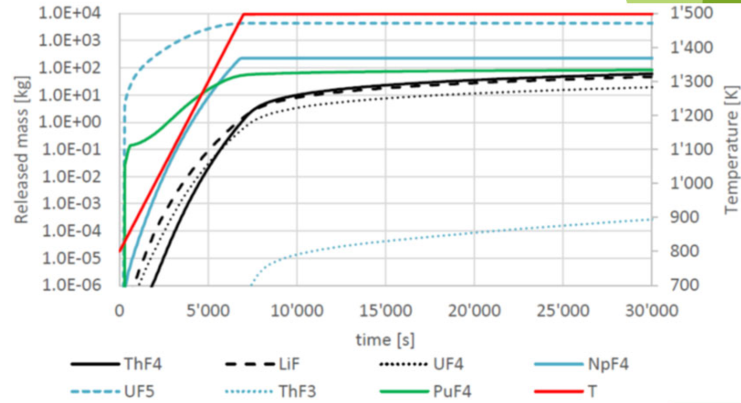
Total released mass during the accidental salt heat up.

Task 3.4: released mass sensitivity to redox

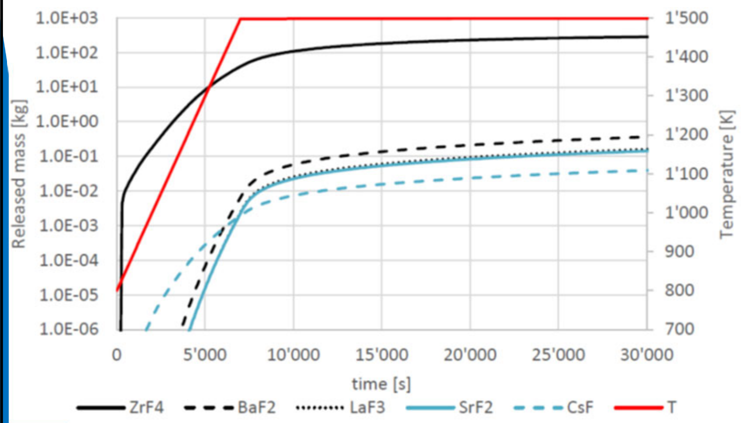
Fluorine: -1% mol. | **Stoichiometric** | **+1% mol.**

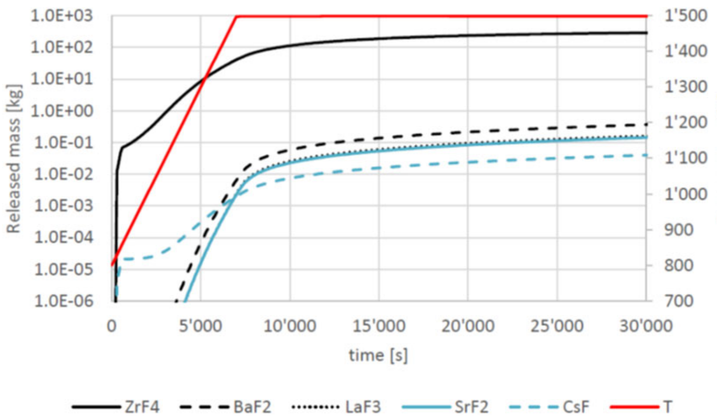


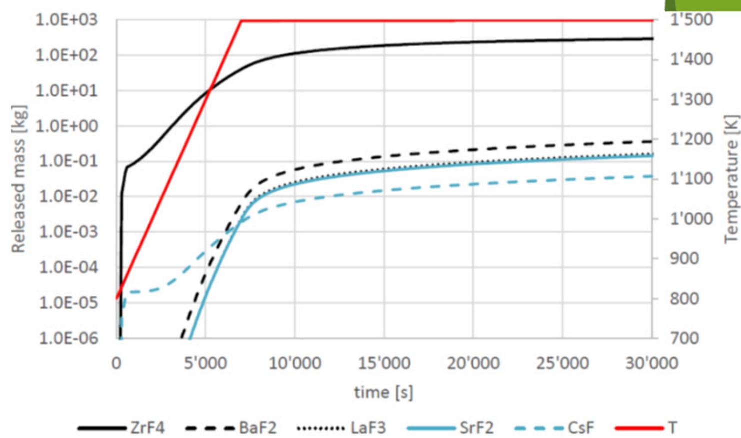




Actinides and salt species





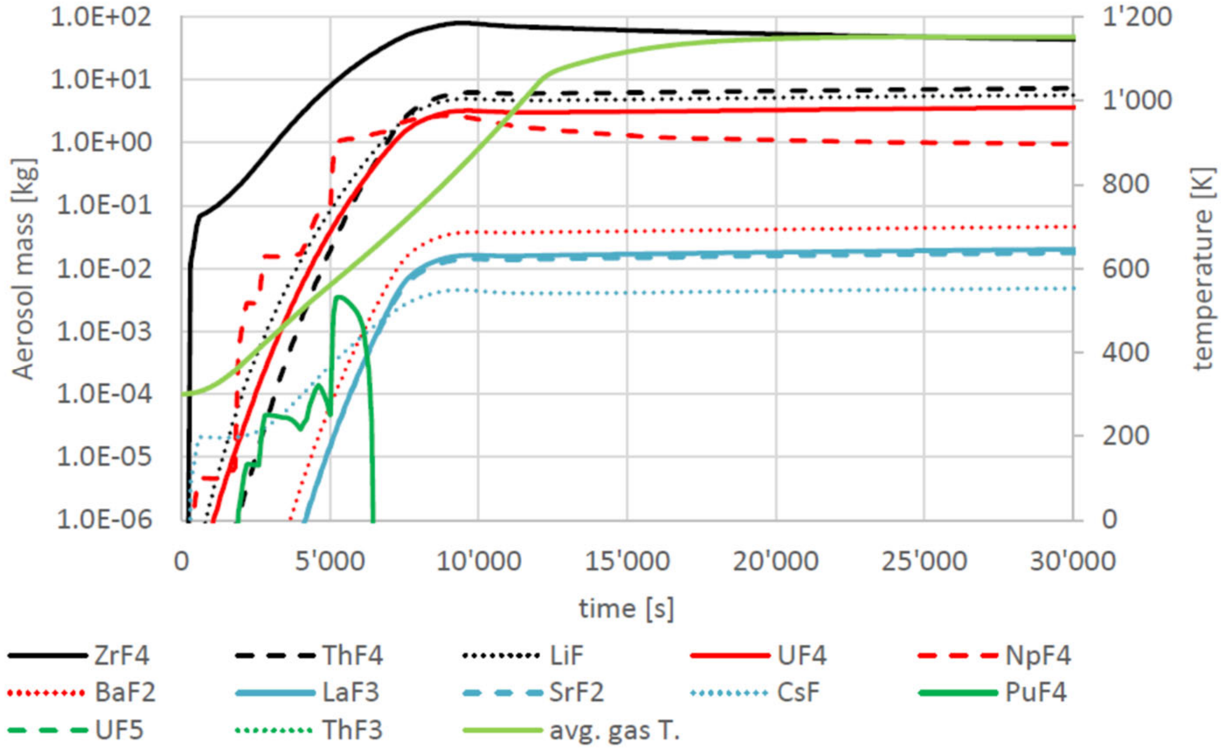


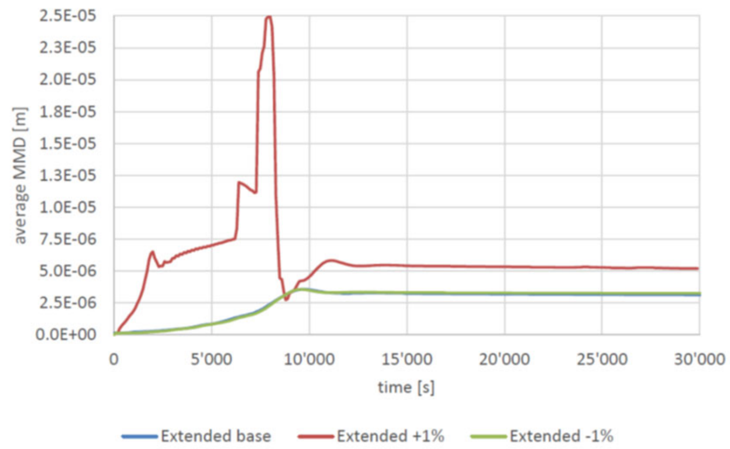
Fission products species

Total released mass during the accident.

Task 3.4: released aerosols mass (cGEMS)

- Characterization of released aerosols





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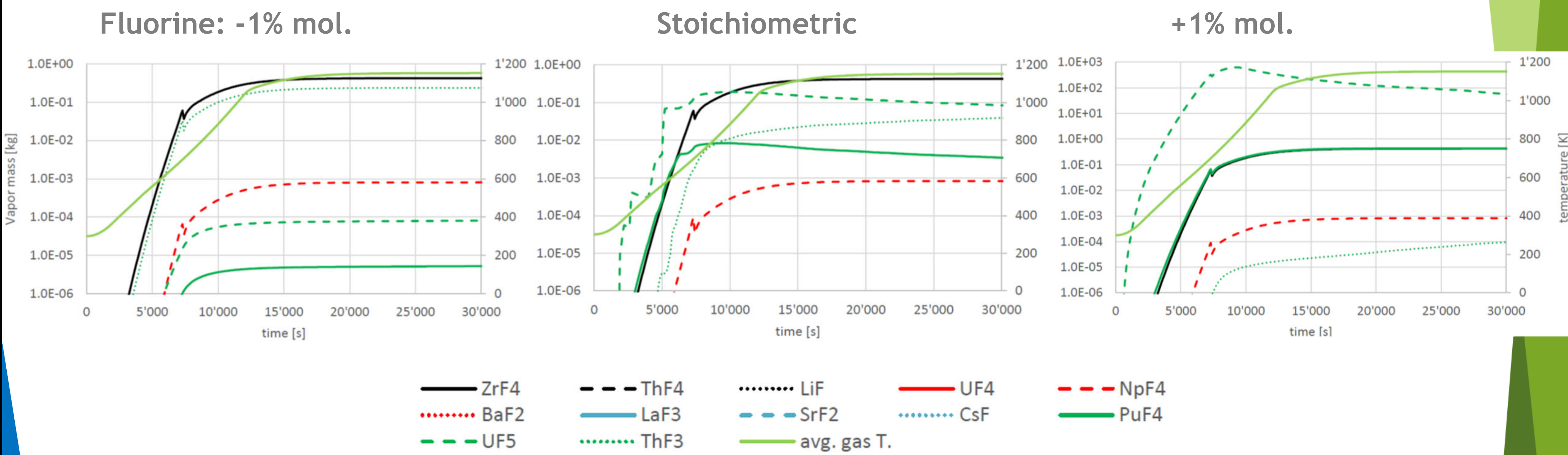
Total released mass of aerosols and their mass median diameter (MMD) during the accident.

Task 3.4: released vapors mass (cGEMS)

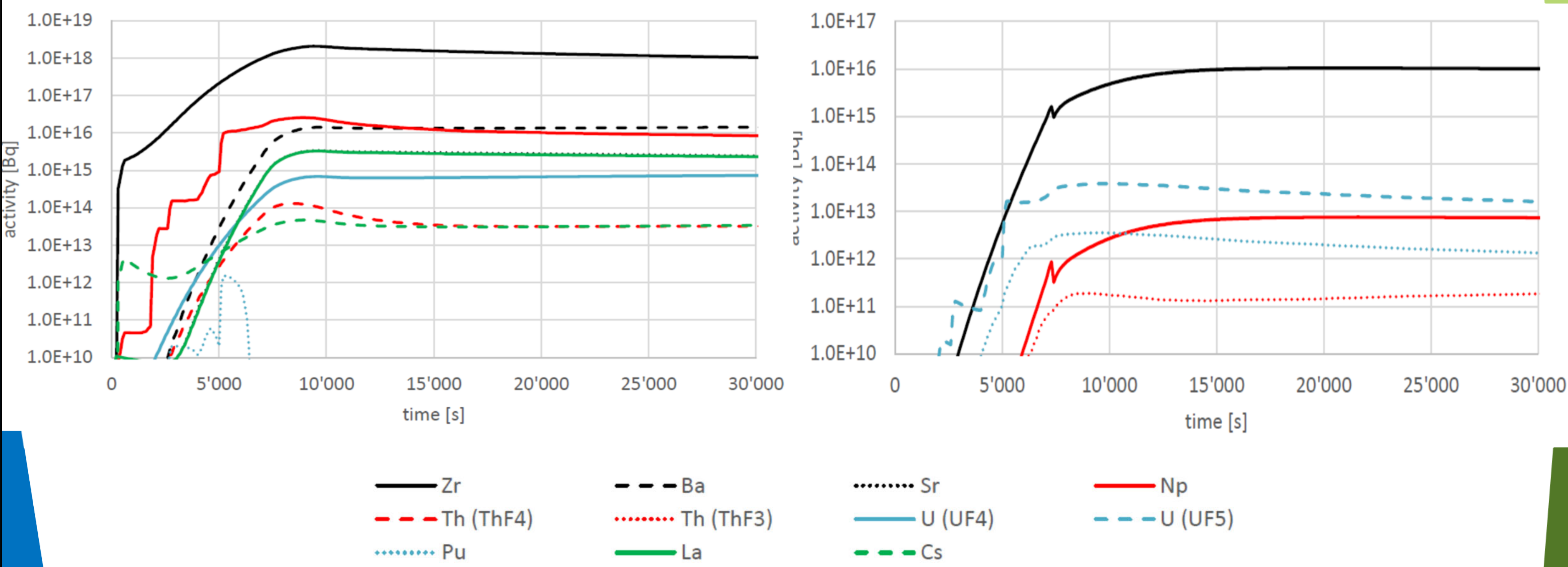
- Characterization of released vapors



Total released mass of vapors during the accident.

Task 3.4: released activity (cGEMS)

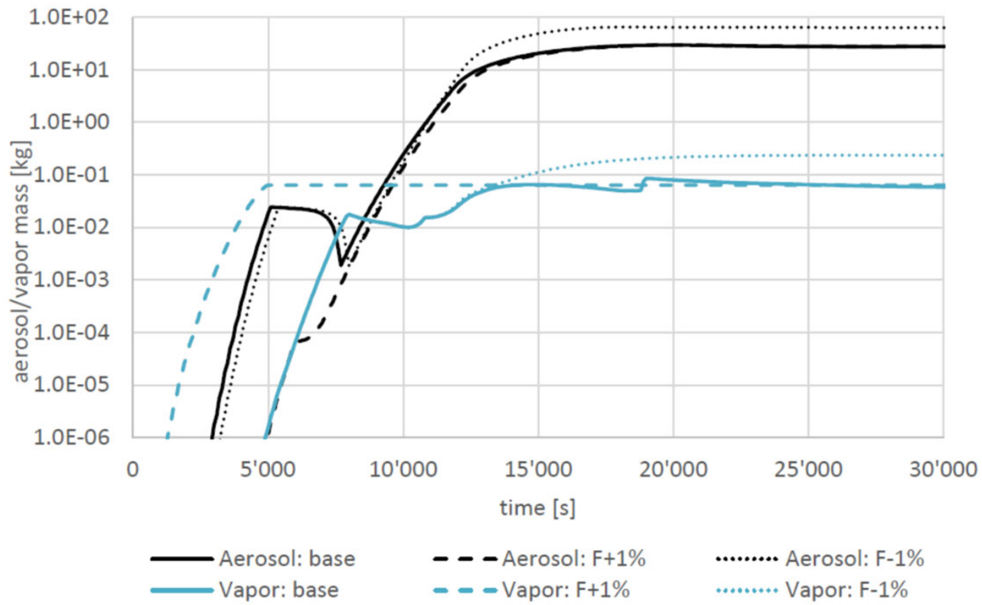
- Characterization of released activity in form of aerosols and vapors



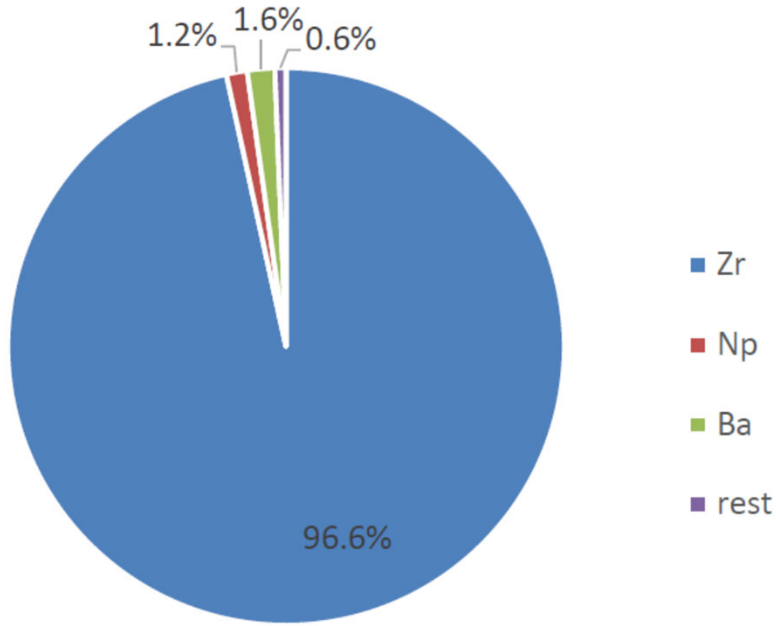
Total released activity in form of aerosols (left) and vapors (right) during the accident.

Task 3.4: conclusion

- Accidental condition behavior and nominal condition removal rates are interconnected.
- Based on the original reprocessing scheme, ZrF_4 in form of aerosols seems to be the major activity carrier during the postulated accident.
- In the updated reprocessing scheme, ZrF_4 removal rate was increased.
- In general, nominal and severe conditions simulation should iterate between each other.



Total released activity in form of aerosols and vapors during the accident.



Activity break-down at the end of simulation (t=30’000s) of the accident.

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Task 3.1: Source term distribution

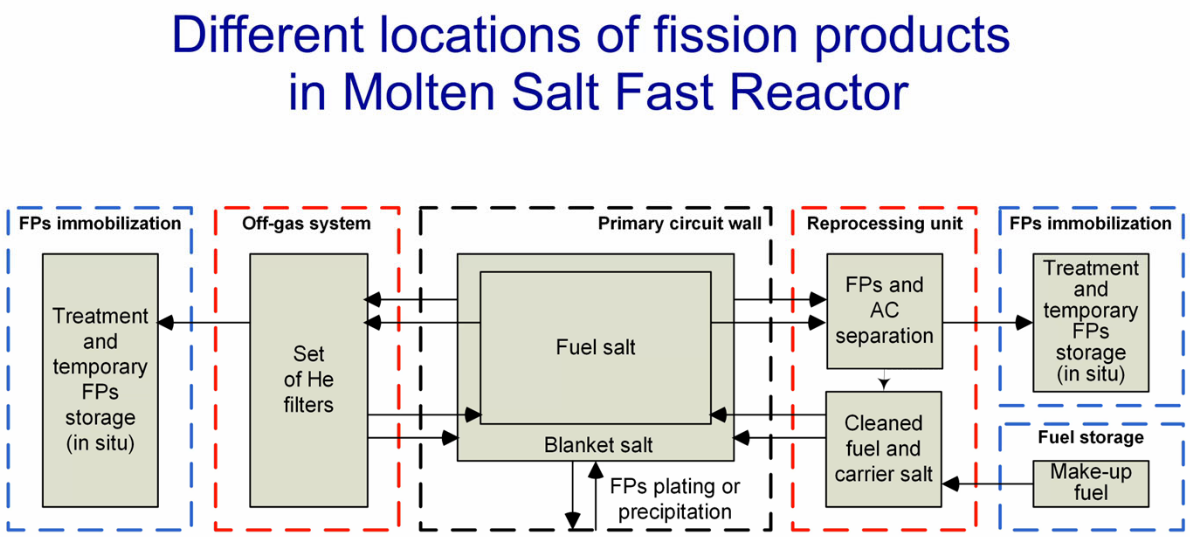
Jiri Krepel (PSI), Lydie Giot (Subatech), Stefano Lorenzi (POLIMI)

SAMOSAFER Final Meeting

28 November 2023, Avignon, France

Task 3.1: overview

- It should provide distribution of nuclides in all locations of the MSFR system.
- This is relatively easy to simulate with high precision.
- However, it may get complicated when many locations are modelled simultaneously. It may require solution of single big matrix 10000+ X 10000+.
- All simulations were based on Serpent 2 code, where Subatech and POLIMI relied on internal Serpent 2 burnup model modified for MSR.
- PSI used Serpent 2 code coupled to MATLAB based routine EQL0D, which enables burnup matrixes modifications, interconnections and complex systems simulations.
- 8 cross-section libraries were used in the simulations: ENDF/B-VIII.0, ENDF/B-VII.1, ENDF/B-VII.0, ENDF/B-VI.8, JEFF-3.3, JEFF-3.11, JEFF-3.1, and JEF-2.2.



Major changes in removal rates

- T3.2: metallic FPs have removal rate 140x longer than gaseous FPs.
- T3.4: Zr is added to the elements, which are removed by off-gas system. Since it has 2.5x lover transfer coefficient in the reprocessing unit, the respective cycle time is 350x longer than for gaseous FPs.
- T3.3: transfer coefficients in the reprocessing plant indicate that each element will have different efficiency of removal.
- As a consequence, Ac losses are explicitly simulated and many FPs have much longer cycle time.

GFPs cycle time [s]	GFPs cycle time [min]	Helium mass flow rate [g/s]	SFPs cycle time [min]	SFPs cycle time [s]
15	0.25	56.4	35	2100
30	0.5	27.8	70	4200
60	1	13.7	140	8400
120	2	6.8	280	16800
240	4	3.3	560	33600
480	8	1.6	1120	67200
960	16	0.81	2240	134400
1920	32	0.40	4480	268800
3840	64	0.20	8960	537600
7680	128	0.10	17920	1075200

Element	WS1	Fluor.	WS2	LME1	LME2	WS3	LMRE	Storage2	Effective cycle time Fuel salt	Effective cycle time Blanket salt
H	1	0	0	0	0	0	0	0	450	18250
He	1	0	0	0	0	0	0	0	450	18250
Li	0	1	0	1	1	0	1	1	Not rem.	Not rem.
Be	0	1	0	1	0.85	0.255	0.745	0.745	1765	71581
B	0.98	0.02	0.02	0	0	0	0	0	450	18250
C	0.5	0.5	0.495	0.005	5E-05	4.95E-05	0.004951	0.004951	452	18331
N	1	0	0	0	0	0	0	0	450	18250
O	0	1	1	0	0	0	0	0	450	18250
F	0	1	0	1	1	0	1	1	Not rem.	Not rem.
Ne	1	0	0	0	0	0	0	0	450	18250
Na	0	1	0	1	0.97	0.58976	0.41024	0.41024	763	30944
Mg	0	1	0	1	0.01	0.0099	0.9901	0.9901	45455	1843453
Al	0	1	0	1	0.01	0.00999	0.99001	0.99001	45045	1826825
Si	0.9	0.1	0.099	0.001	0	0	0.001	0.001	450	18250
P	1	0	0	0	0	0	0	0	450	18250
S	0.9	0.1	0.099	0.001	0.001	0	0.001	0.001	450	18250
Cl	0	1	0.99	0.01	0.01	0	0.01	0.01	455	18453
Ar	1	0	0	0	0	0	0	0	450	18250
K	0	1	0	1	0.98	0.49588	0.50412	0.50412	907	36784
Ca	0	1	0	1	0.1	0.099	0.901	0.901	4545	184325
Sc	0	1	0	1	0.8	0.56	0.44	0.44	804	32607
Ti	0	1	0.99	0.01	0	0	0.01	0.01	455	18453
V	0	1	0.99	0.01	0.0001	9.99E-05	0.0099	0.0099	454	18412
Cr	0	1	0.99	0.01	0.0001	9.99E-05	0.0099	0.0099	454	18412
Mn	0	1	0.99	0.01	0.0001	9.99E-05	0.0099	0.0099	454	18412
Fe	0	1	0	1	0.01	0.00999	0.99001	0.99001	45045	1826825
Co	0.5	0.5	0.25	0.25	0.0025	0.002498	0.247503	0.247503	598	24252
Ni	0.5	0.5	0	0.5	0.005	0.004995	0.495005	0.495005	891	36135
Cu	0.5	0.5	0	0.5	0.005	0.004995	0.495005	0.495005	891	36135
Zn	0.5	0.5	0	0.5	0.005	0.004995	0.495005	0.495005	891	36135
Ga	0.5	0.5	0.495	0.005	5E-05	5E-05	[illegible]	[illegible]	452	18331
Ge	0.5	0.5	0.495	0.005	5E-05	[illegible]	[illegible]	[illegible]	[illegible]	18331

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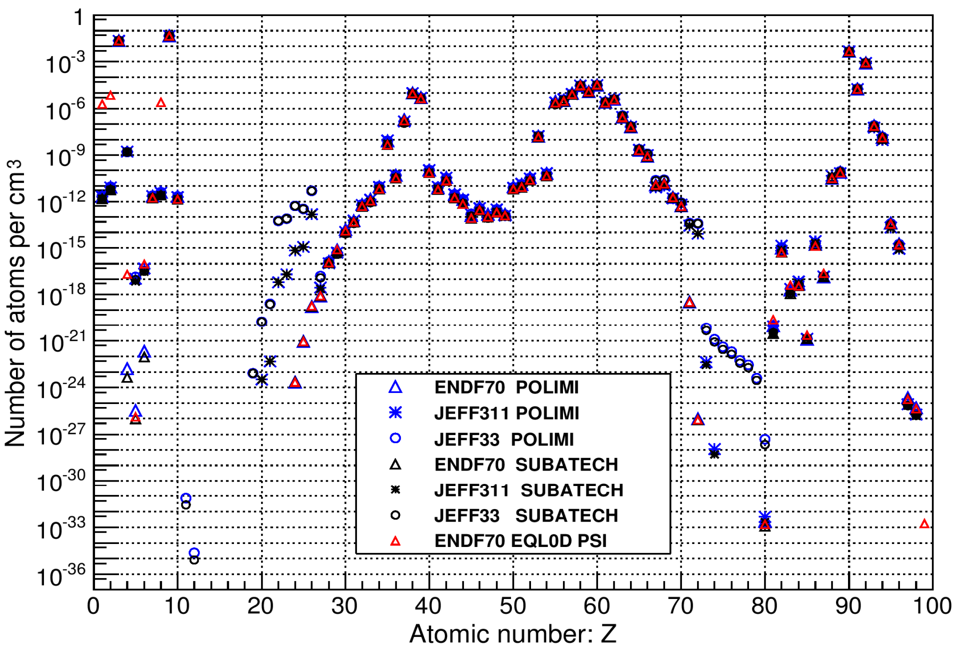
Benchmark of the tools

- There are differences between the tools, but also between the libraries.
- The overall distribution is similar. However, for some less populated nuclides there are differences.



Nuclides concentration after 5 EFPD irradiation grouped per atomic number Z.

Nuclides concentration after 20 EFPY irradiation compared to ENDF/B-VIII.0 results.

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Benchmark of the tools

- There are differences between the tools, but also between the libraries.
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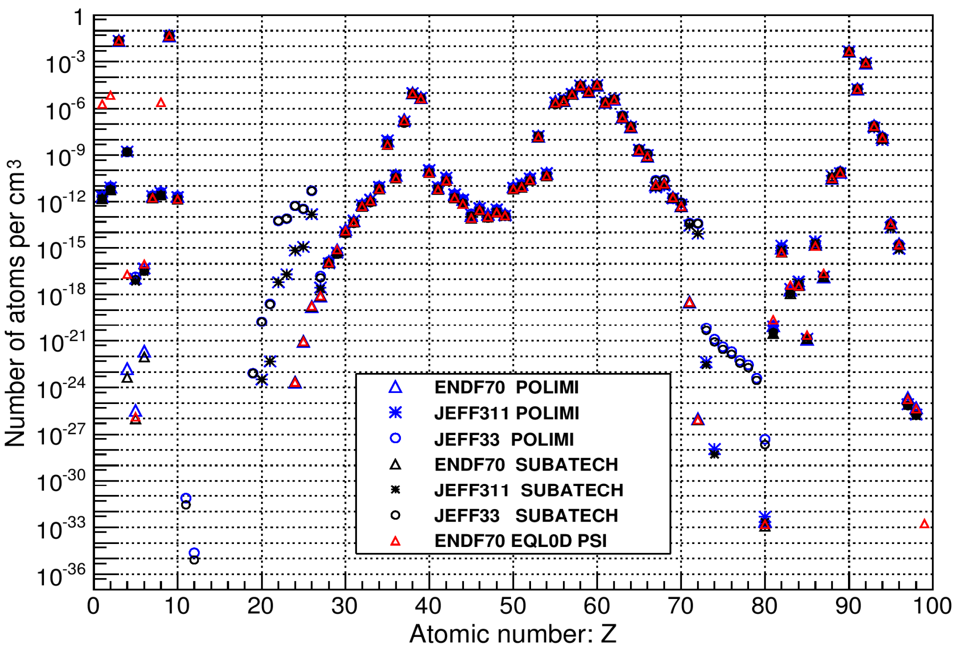
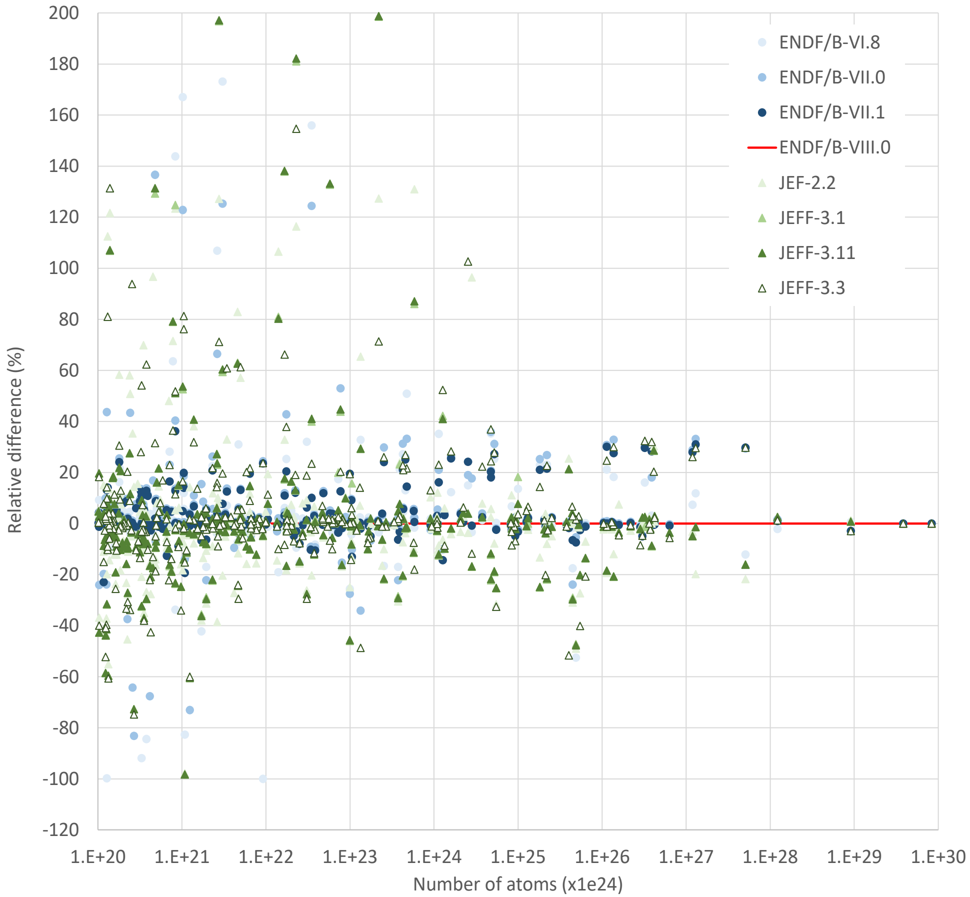


Nuclides concentration after 5 EFPD irradiation grouped per atomic number Z.



Nuclides concentration after 20 EFPY irradiation compared to ENDF/B-VIII.0 results in (%).

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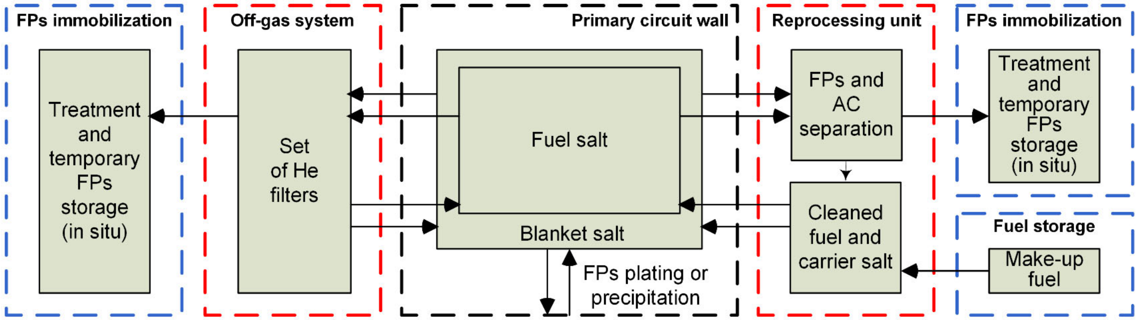
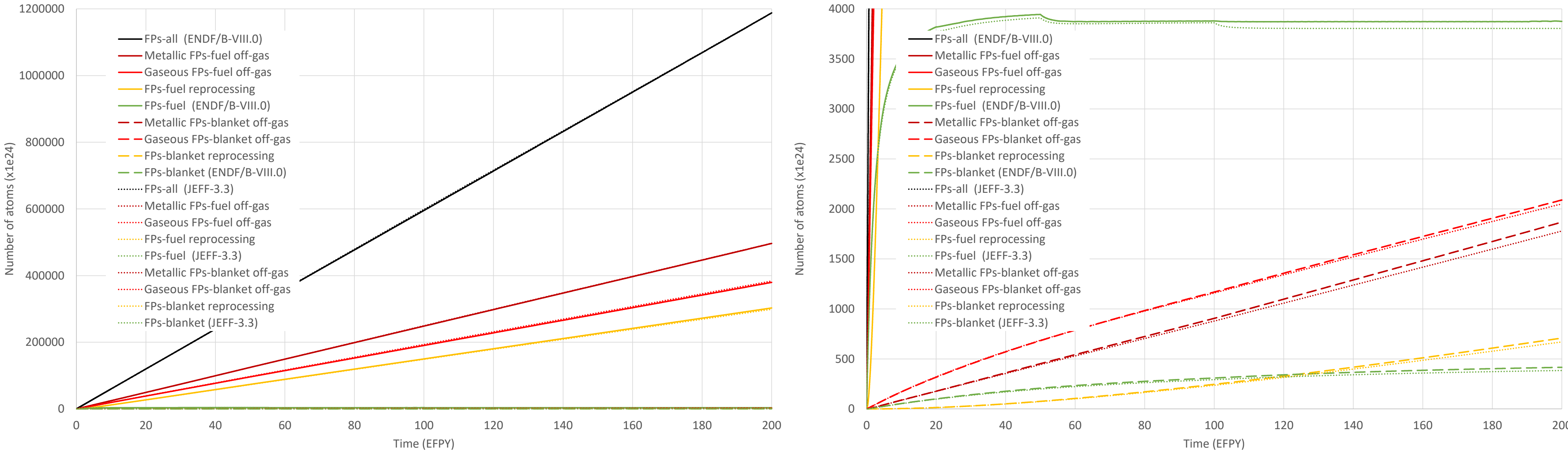
FPs mass evolution in MSFR systems

- When whole MSFR system is simulated the FPs cumulate in the off-gas system and reprocessing unit.

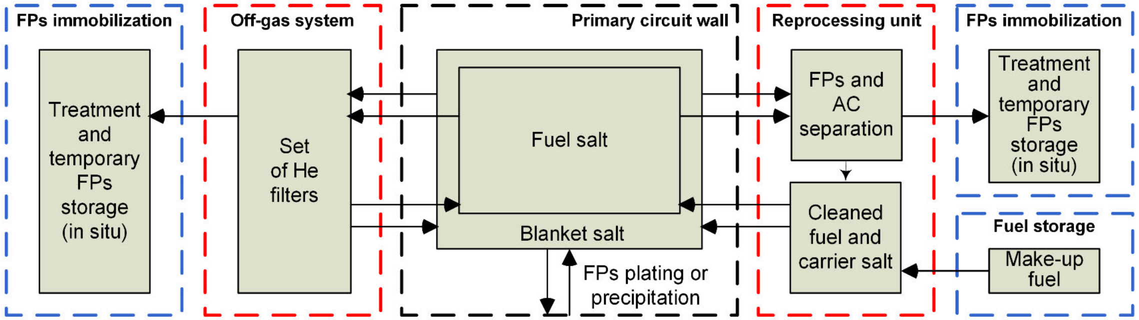


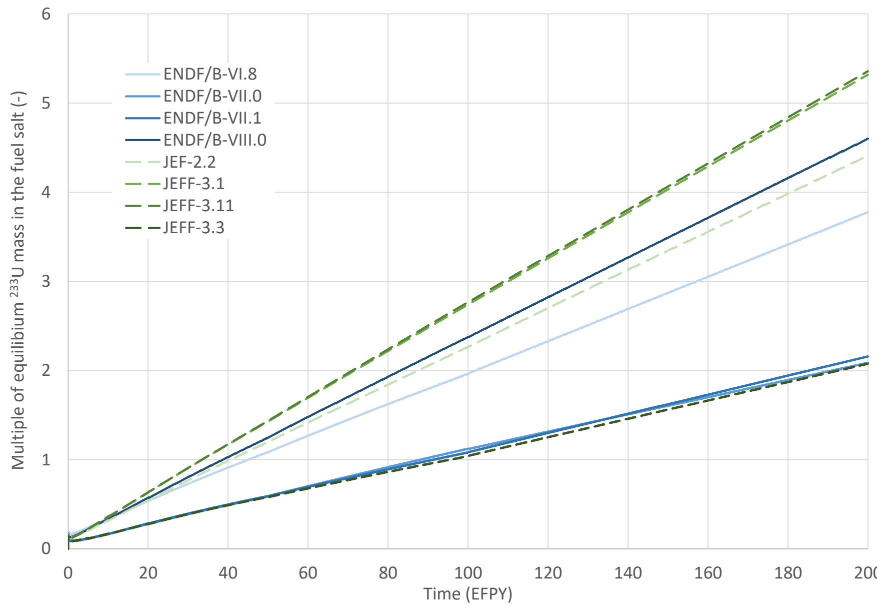


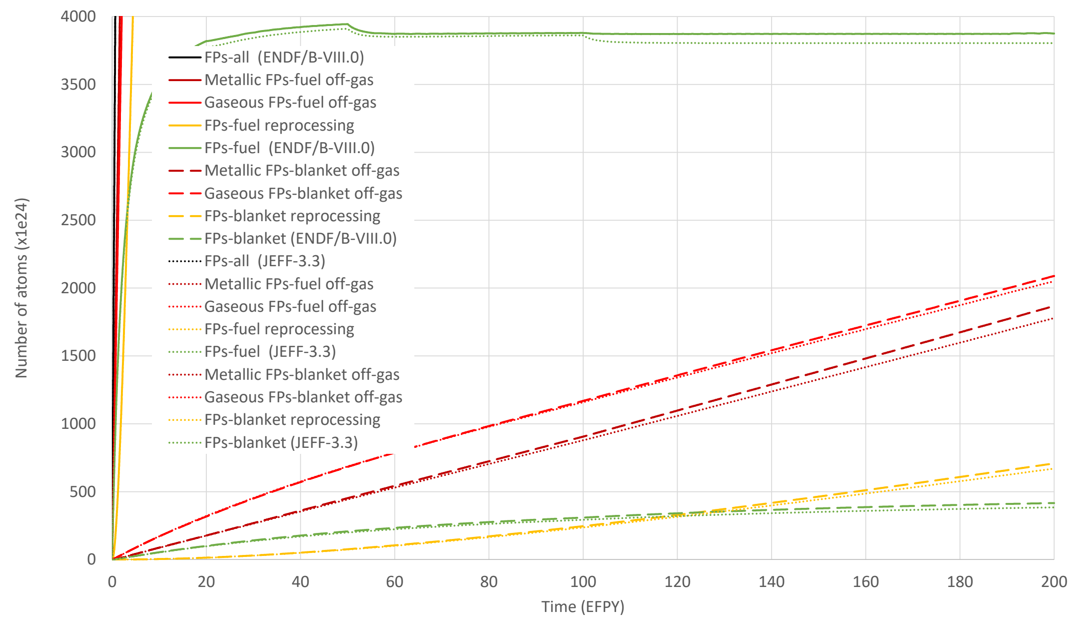
FPs atoms in different MSFR system locations for ENDF/B-VIII.0 and JEFF-3.3 cross-section libraries.

FPs mass evolution in MSFR systems

- When whole MSFR system is simulated the FPs cumulate in the off-gas system and reprocessing unit.
- Doubling time strongly differs.







FPs atoms in different MSFR system locations for ENDF/B-VIII.0 and JEFF-3.3 cross-section libraries.

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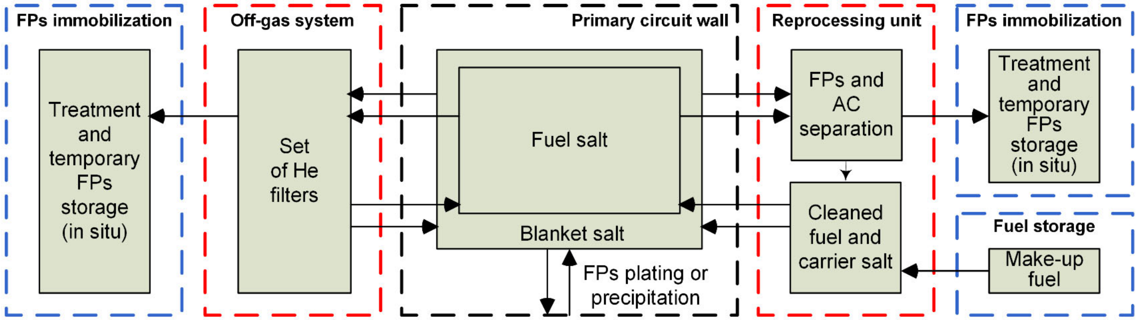
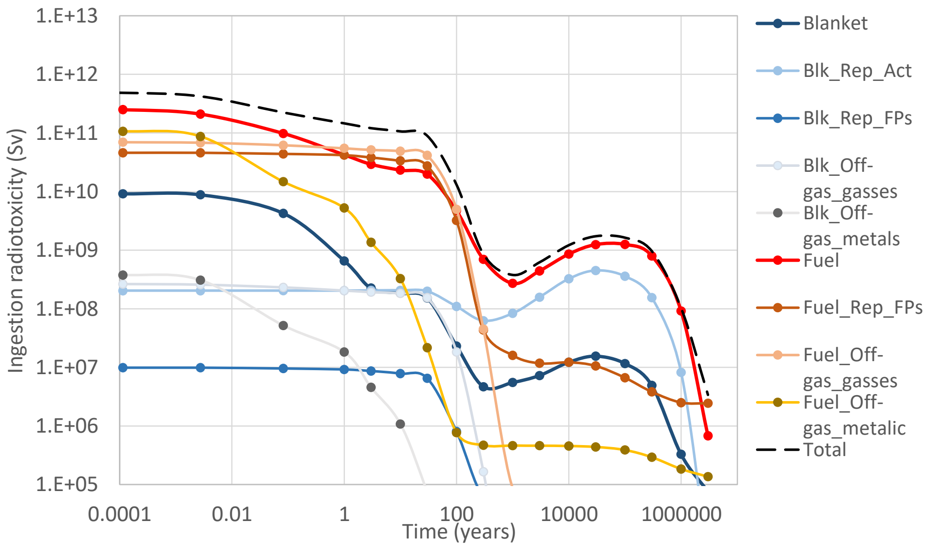
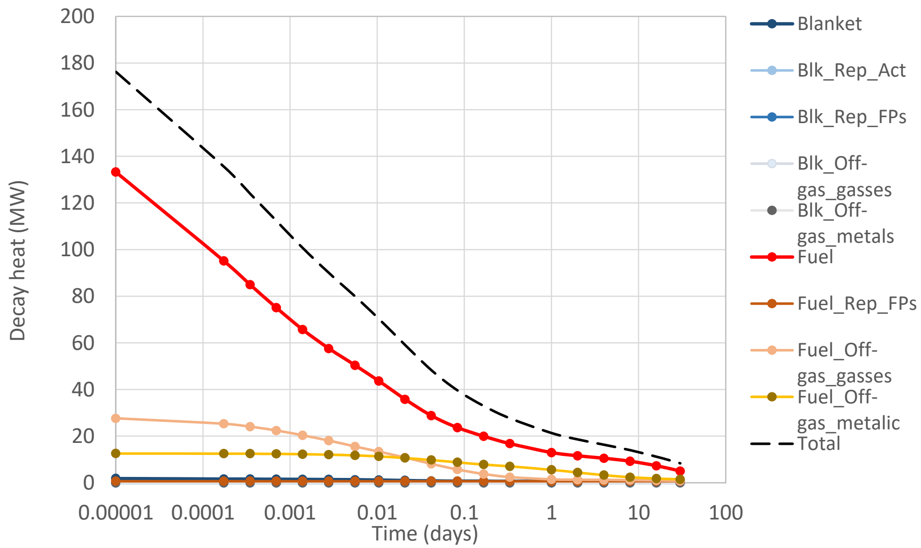
FPs mass evolution in MSFR systems

- Radiotoxicity and decay heat distribution after 20 EFPY of operation.





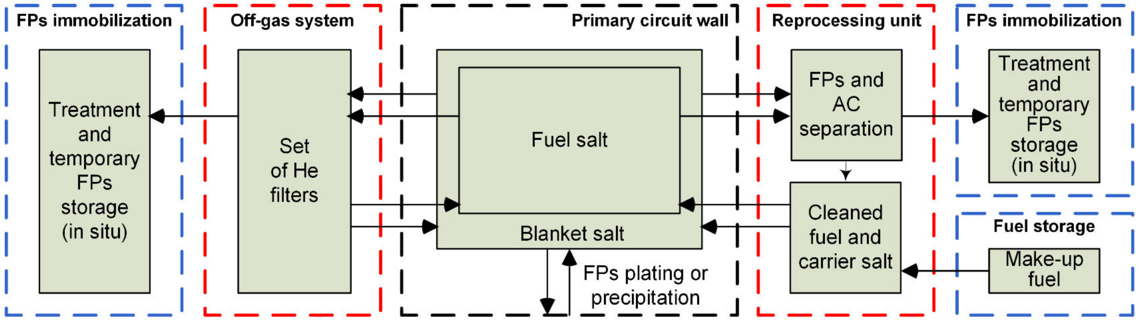
Distribution of ingestion radiotoxicity between several locations (Blk. – blanket salt, Fuel – fuel salt, Rep. –reprocessing unit) after 20 EFPY of irradiation.



Distribution of decay heat between several locations (Blk. – blanket salt, Fuel – fuel salt, Rep. –reprocessing unit) after 20 EFPY of irradiation.

FPs mass evolution in MSFR systems

- Top 15 decay chains (the same A) according to ingestion radiotoxicity.
- The off-gas system dominates in many cases.



Rank	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
Atomic number	233	131	90	137	140	133	144	91	132	89	143	97	95	93	141
Nuclides	233Th 233Pa	131Cd 131In 131Sn 131Sb 131Te-m 131Te 131I 131Xe-m	90Se 90Br 90Kr 90Rb-m 90Rb 90Sr 90Y	137Sn 137Sb 137Te 137I 137Xe 137Cs 137Ba-m	140Te 140I 140Xe 140Cs 140Ba 140La	133In 133Sn 133Sb 133Te-m 133Te 133I 133Xe-m 133Xe	144Xe 144Cs 144Ba 144La 144Ce 144Pr-m 144Pr 144Nd	91Se 91Br 91Kr 91Rb 91Sr 91Y	132In 132Sn 132Sb-m 132Sb 132Te 132I 132Xe 132Cs	89As 89Se 89Br 89Kr 89Rb 89Sr 89Y-m	143Xe 143Cs 143Ba 143La 143Ce 143Pr 143Nd	97Kr 97Rb 97Sr 97Y 97Zr 97Nb-m 97Nb	95Kr 95Rb 95Sr 95Y 95Zr 95Nb-m 95Nb 95Mo	93Br 93Kr 93Rb 93Sr 93Y 93Zr 93Nb-m	141I 141Xe 141Cs 141Ba 141La 141Ce
Half-lives	22m 27d	0.106s 0.28s 39s 23.0m 1.35d 25.0m 8.040d 11.9d	0.427s 1.9s 32.3s 4.3m 2.6m 29.1y 2.67d	- 0.478s 2.5s 24.5s 3.82m 30.17y 2.552m	0.894s 0.86s 13.6s 1.06m 12.75d 1.678d	0.18s 1.44s 2.5m 55.4m 12.4m 20.8h 2.19d 5.243d	1.2s 1.01s 11.4s 40.7s 284.6d 7.2m 17.28m 15.32l	0.27s 0.54s 8.6s 58.0s 9.5h 58.5d	0.20s 40s 2.8m 4.2m 3.26d 2.28h stable 6.475d	0.121s 0.41s 4.37s 3.15m 15.4m 50.52d 15.7s	0.30s 1.78s 14.3s 14.1m 1.38d 13.57d stable	0.1s 0.169s 0.42s 3.76s 16.8h 58.1s 1.23h	0.78s 0.377s 25.1s 10.3m 64.02d 3.61d 34.97d stable	0.176s 1.29s 5.85s 7.4m 10.2h 1.5e6y 12y	0.45s 1.72s 24.9s 18.3m 3.90h 32.50d
Total ingestion radiotoxicity (Sv)	**9.2E+10**	**7.7E+10**	**7.3E+10**	**3.0E+10**	**2.8E+10**	**2.5E+10**	**2.4E+10**	**1.9E+10**	**1.8E+10**	**1.6E+10**	**1.3E+10**	**1.1E+10**	**9.5E+09**	**7.9E+09**	**6.9E+09**
Off-gas system (%)	0.0	**67.0**	**38.3**	**82.1**	**11.0**	**37.7**	0.0	**9.6**	**98.6**	**75.4**	0.0	**89.5**	**97.2**	0.2	0.6
Fuel in core (%)	**90.7**	**32.1**	**20.6**	2.1	**88.1**	**61.9**	**66.2**	**87.7**	1.4	**23.8**	**98.2**	**10.5**	2.8	**99.4**	**95.7**
Reprocessing unit (%)	0.1	0.8	**40.9**	**15.8**	0.5	0.2	**33.4**	2.3	0.0	0.8	1.4	0.0	0.0	0.0	3.4
Fuel in blanket (%)	**9.2**	0.1	0.2	0.1	0.3	0.2	0.4	0.3	0.0	0.1	0.4	0.0	0.0	0.4	0.4

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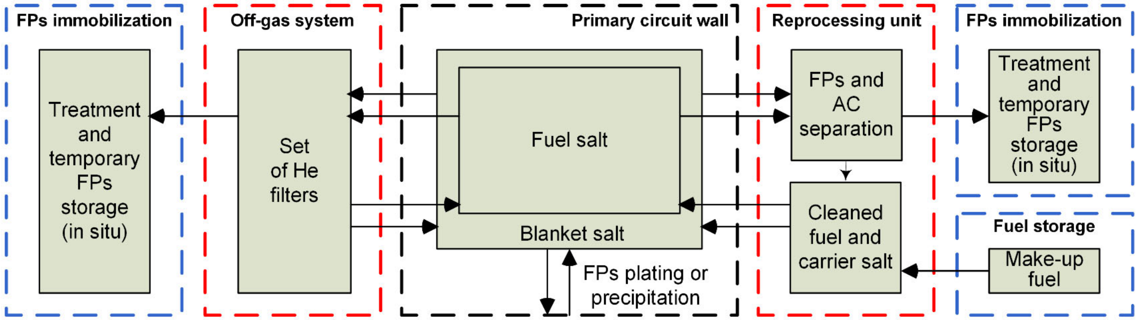
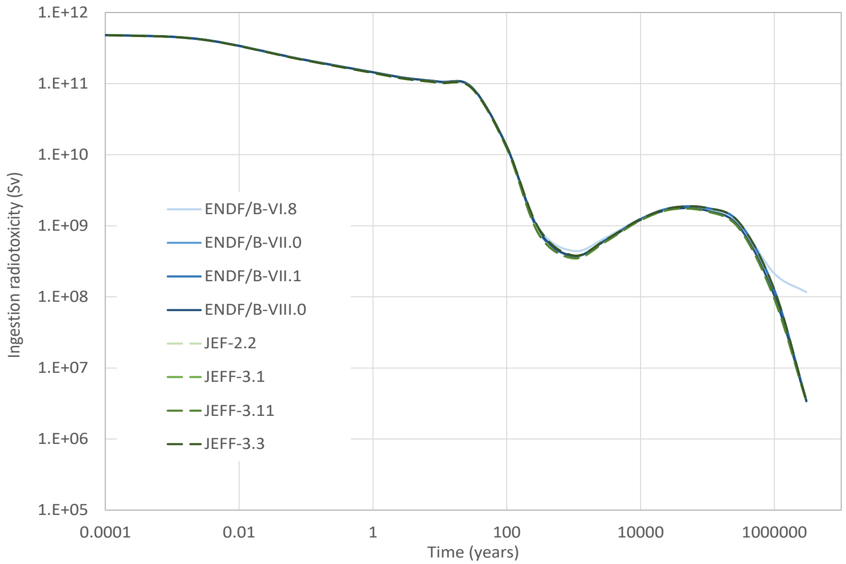
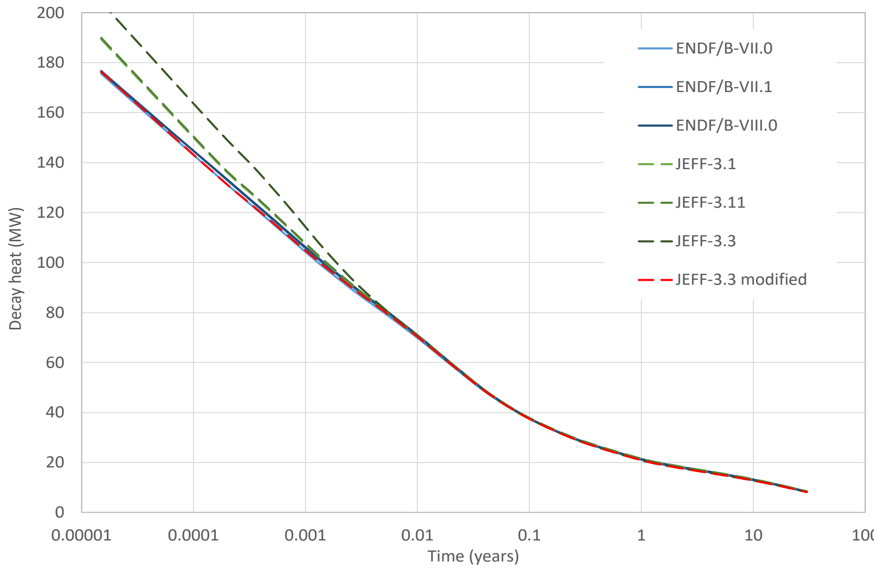
FPs mass evolution in MSFR systems

- Radiotoxicity and decay heat distribution after 20 EFPY of operation.





Total ingestion radiotoxicity for different libraries after 20 EFPY of irradiation.



Total decay heat for different libraries after 20 EFPY of irradiation.

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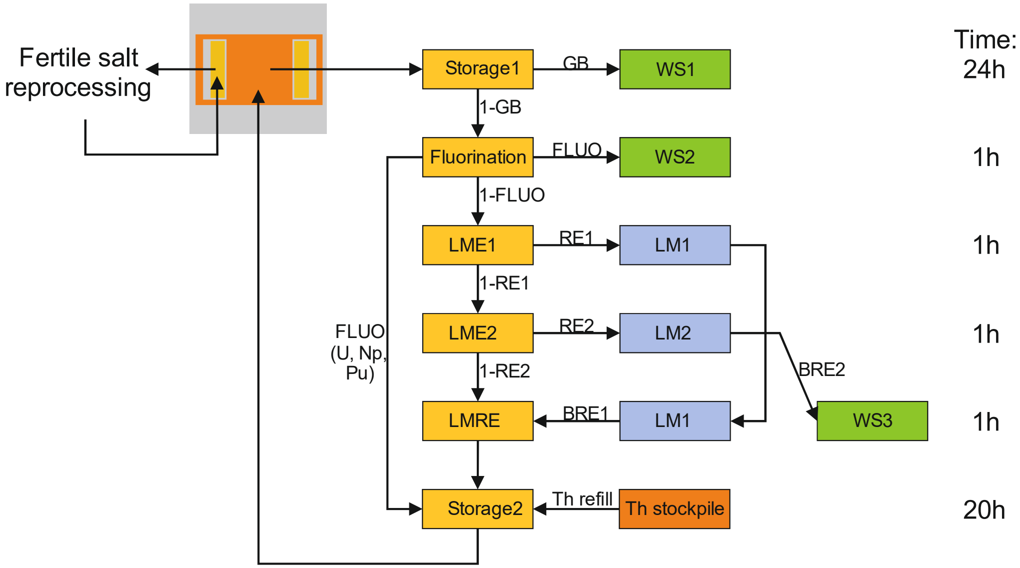
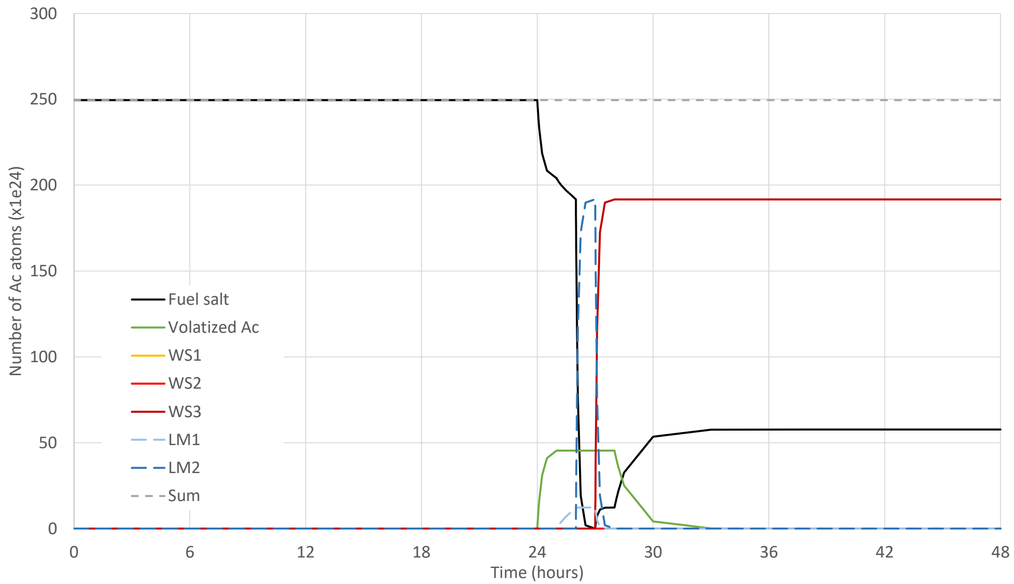
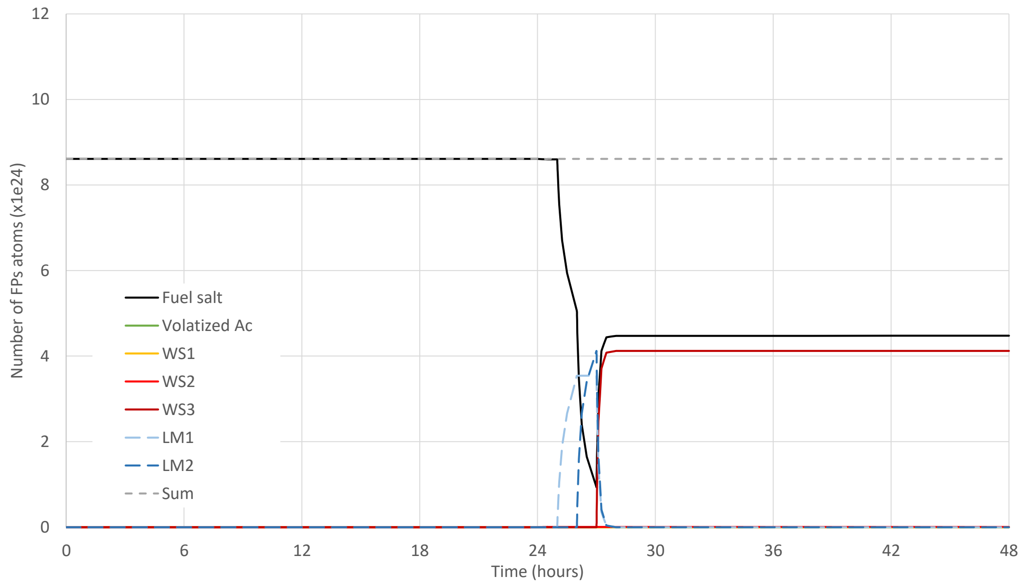
FPs mass evolution in reprocessing systems

- Ac and FPs flow through the reprocessing unit.
- Th fully removed, whereas many FPs only partially.





Distribution of Ac during the 48 hours of salt residence time in in reprocessing unit.



Distribution of FPs during the 48 hours of salt residence time in in reprocessing unit.

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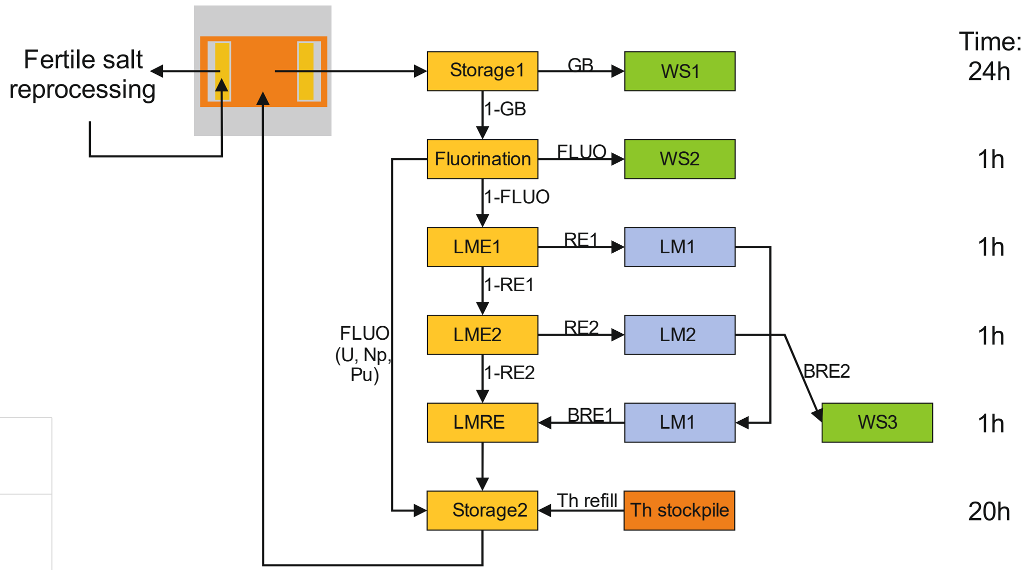
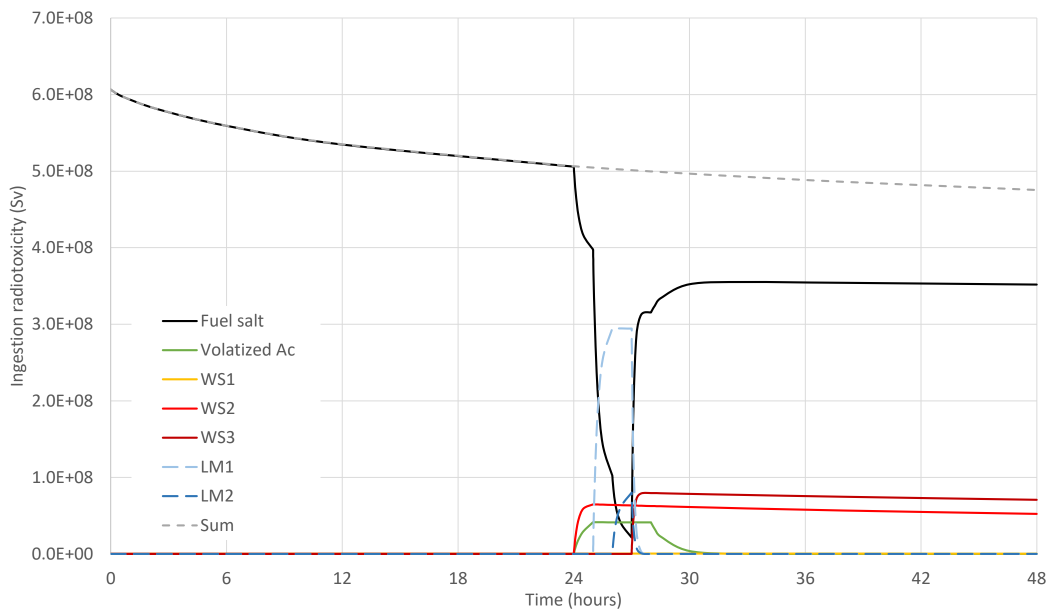
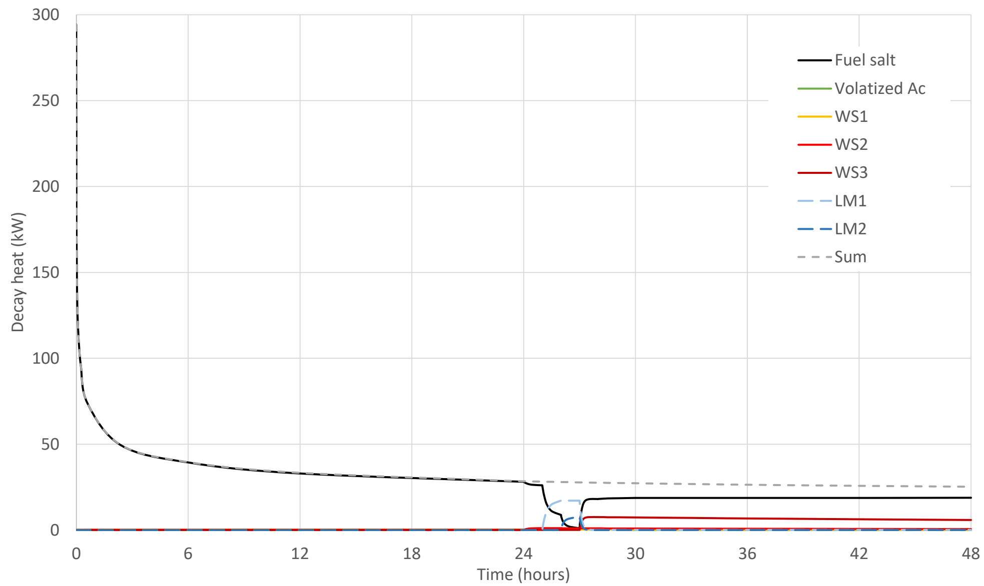
FPs mass evolution in reprocessing systems

- Decay heat and radiotoxicity distribution in the MSFR reprocessing system.





Distribution of ingestion radiotoxicity during the 48 hours of salt residence time in reprocessing unit.



Distribution of decay heat during the 4 hours of salt processing.

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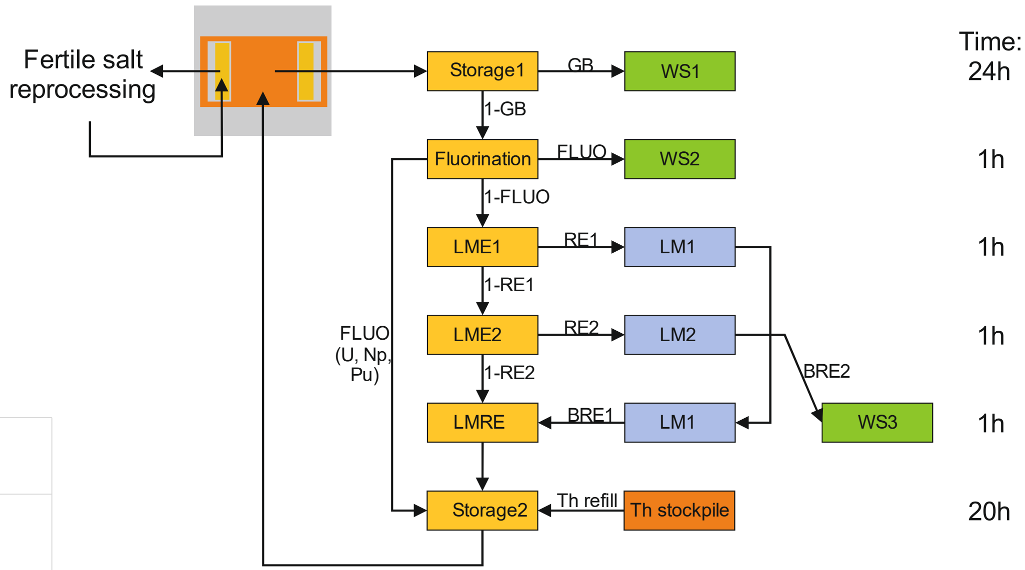
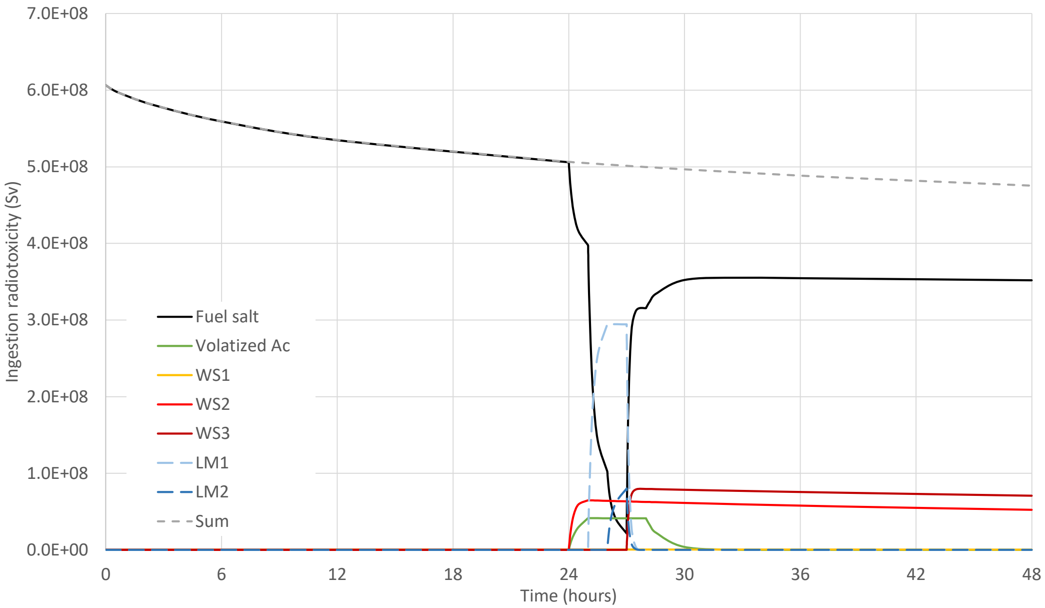
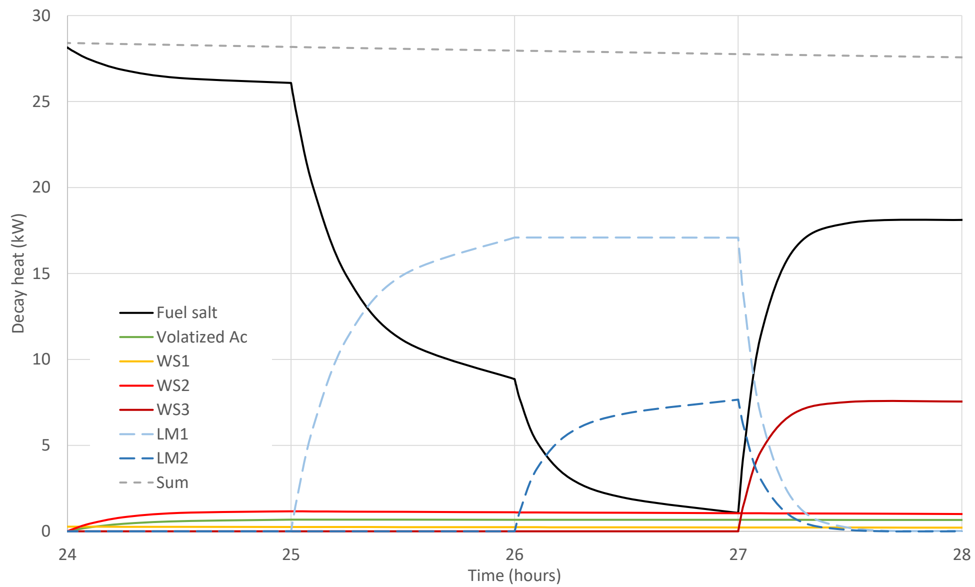
FPs mass evolution in reprocessing systems

- Decay heat and radiotoxicity distribution in the MSFR reprocessing system.





Distribution of ingestion radiotoxicity during the 48 hours of salt residence time in reprocessing unit.



Distribution of decay heat during the 4 hours of salt processing.

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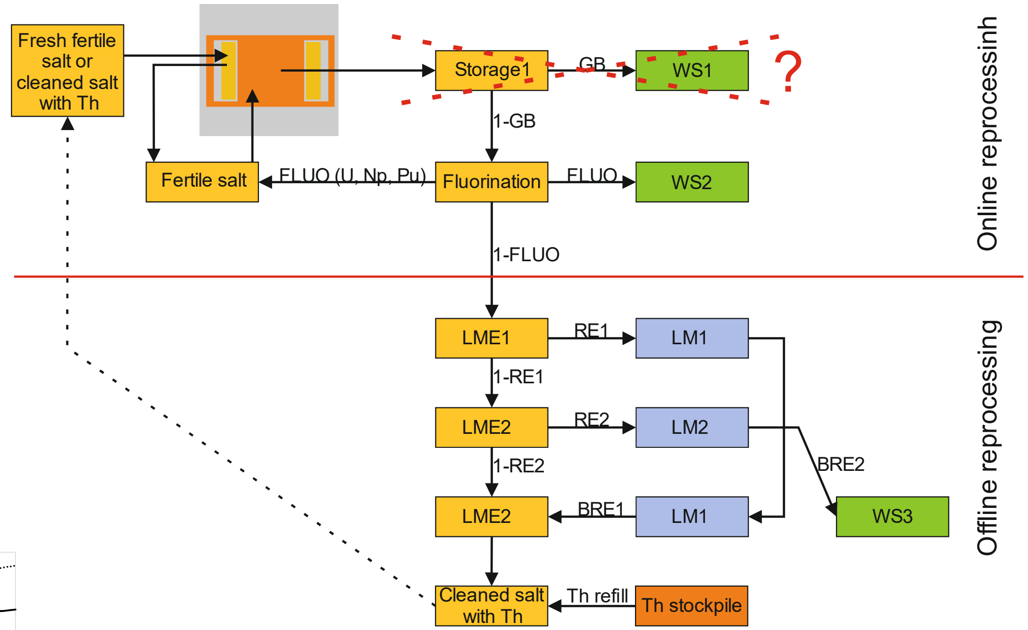
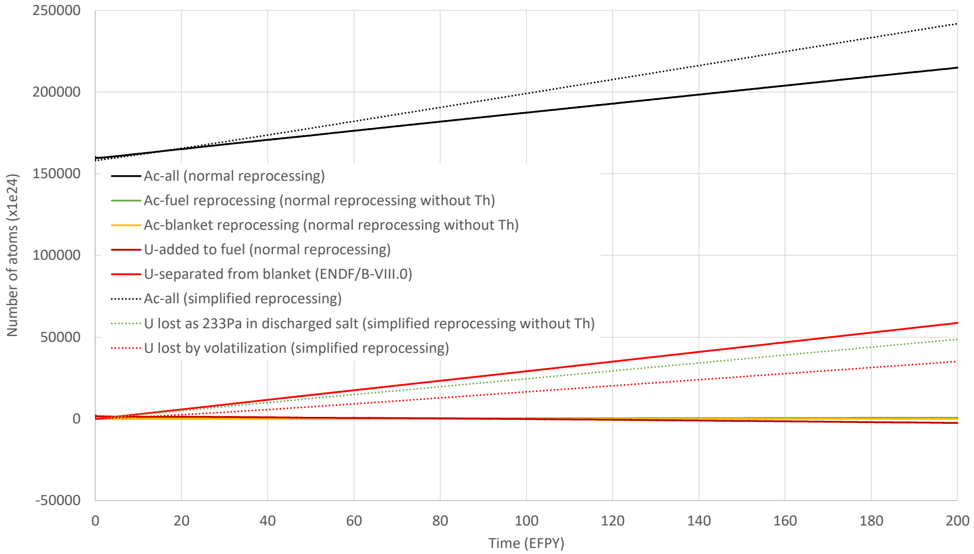
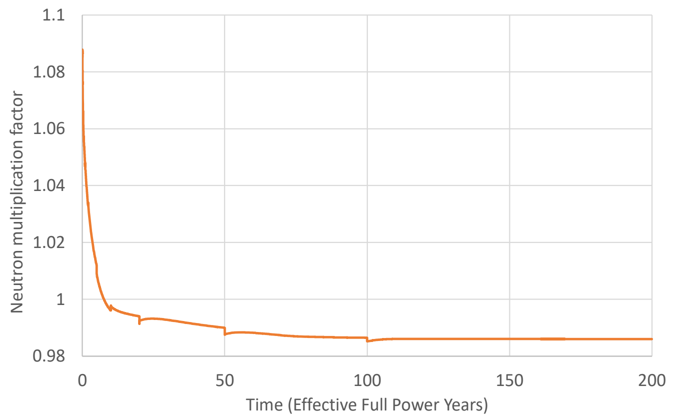
Assessment of simplified reprocessing

- Simplified reprocessing relies only on volatilization in –situ. The rest is done ex-situ.
- Without few months cooling before the actual volatilization, ^{233}U losses through not recycled ^{233}Pa are prohibitive.





Actinides evolution in normal and simplified reprocessing.



Evolution of multiplication factor (without any control).

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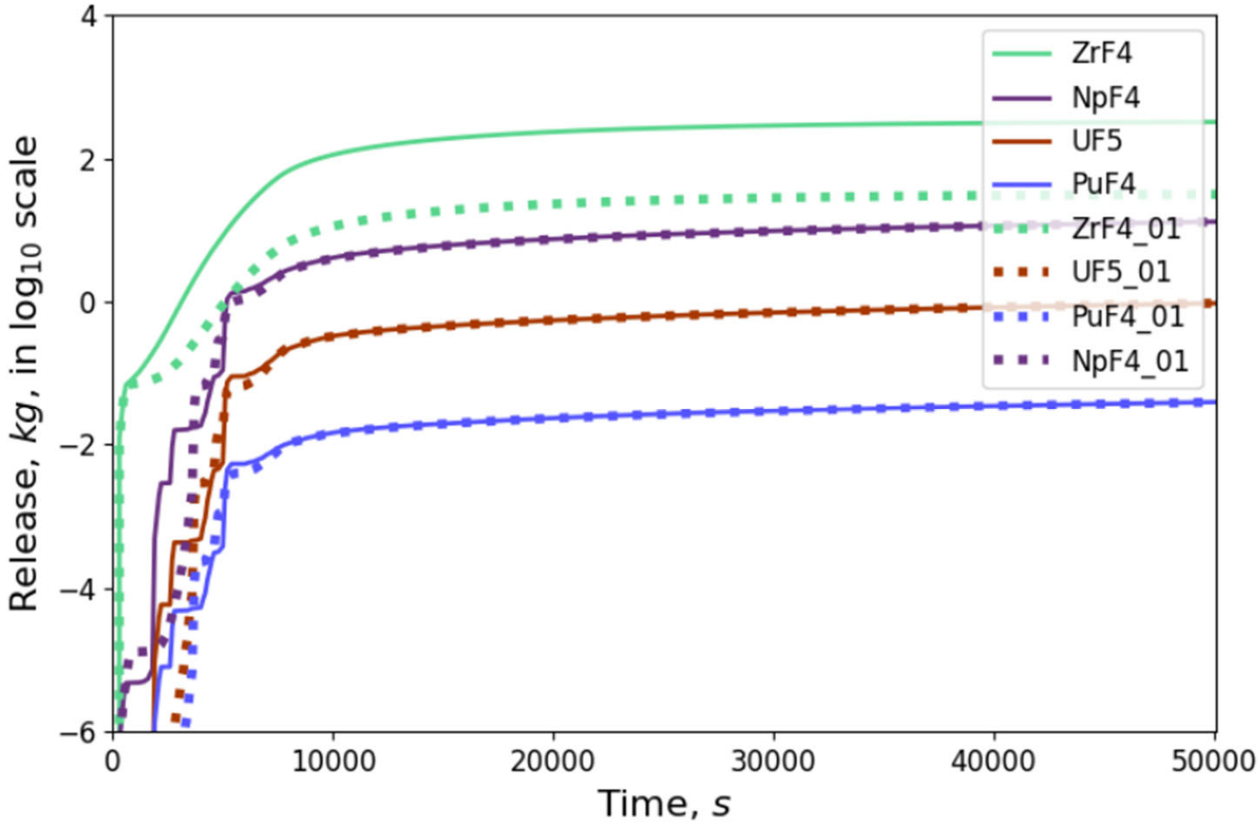
Task 3.1: conclusion

- Differences between libraries and stochastic nature of the cross-section calculations make the tool benchmarking complicated.
- Since size and form of final waste storage is not fully defined, its mass and radiotoxicity cumulated in the off-gas system and reprocessing unit.
- The breeding performance (doubling time) strongly differs between libraries.
- With the explicitly simulated transfer coefficient there are actinides losses in the waste streams.
- Th is so far not recycled and FPs removal efficiency is around 50%.
- The decay heat in the 40l of reprocessed salt after 24 hours of cooling is below 30 kW.
- With updated transfer coefficients the ZrF_4, originally causing major activity release during an accident, is now located in the off-gas system.

Task 3.1 & Task 3.4 provisional iteration

- Comparison of the original calculations of the FP release with the adjusted composition



Total released mass during the accidental salt heat up.

WP3 conclusion and outlook

- **Task 3.2**, based on a complex CFD simulations, identified a ratio of 140 between gaseous and metallic FPs removal rates.
  - **Outlook:** In the future these activities may focus on passive off-gas system without He as working medium (simplicity, safety, economy).
- **Task 3.3** analyzed the major reprocessing techniques and identified a high temperature issue for volatilization and back extraction efficiency for liquid metal extraction. Chloride salt reprocessing scheme and elements valence states were proposed, but without transfer coefficients and residence time.
  - **Outlook:** the transfer coefficients for chlorides salt should be calculated. The reprocessing schemes reviewed and possibly simplified (divided into in-situ and ex-situ parts).
- Task 3.4 provided insight to severe accident behavior, compounds evaporation and formation of gases and aerosols. It also showed, that the containment would be pressurized by air heat up.
  - **Outlook:** further extension of the thermo-dynamics database for fluoride and chloride salts. Iterative approach between fuel burnup calculations, off-gas CFD simulation and severe accident simulations.
- Task 3.1 was acting as an integrating factor and used results from the other task to provide distribution of nuclides, ingestion radiotoxicity and decay heat. It confirmed several weaknesses of the reprocessing scheme and explicitly simulated individual recycling efficiencies.
  - **Outlook:** Application of the methodology on other MSR systems and focusing on the safeguarding of the reprocessing schemes and waste treatment.