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Molten Salt Reactors Taxonomy and Fuel Cycle Performance

Dr. Jiri Krepel
Paul Scherrer Institut

25 January 2023

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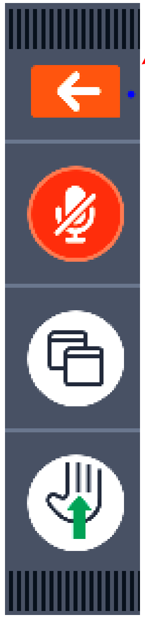

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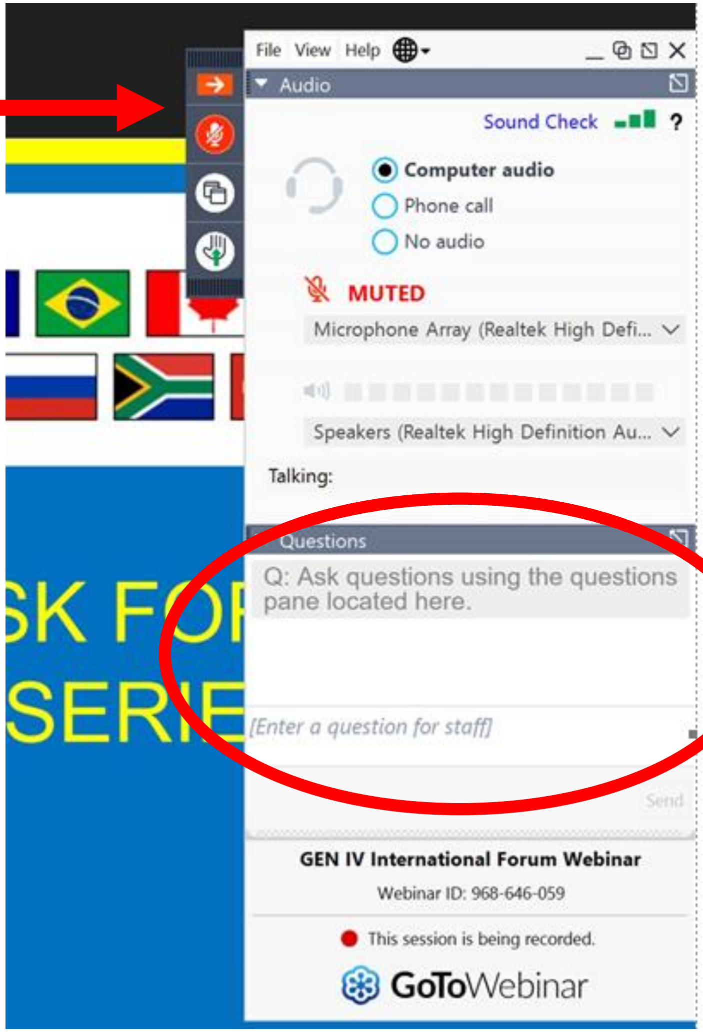

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Meet the Presenter

Dr. Jiri Krepel is a senior scientist in Advanced Nuclear Systems group of Laboratory for Scientific Computing at Paul Scherrer Institut (PSI) in Switzerland and chairman of the Steering Committee of GIF MSR project. He earned his PhD in 2006 at the Czech Technical University (CTU), Prague / Helmholtz-Zentrum Dresden-Rossendorf, Germany for his thesis entitled "Dynamics of Molten Salt Reactors." At PSI, he is the coordinator of the PSI MSR research and responsible for fuel cycle analysis and related safety parameters of Gen IV reactors. He has experience in the neutronics of liquid-metal and gas-cooled fast reactors and in neutronics and transient analysis of thermal and fast MSRs.

Email: jiri.krepel@psi.ch

Outline

I. MSR definition and taxonomy

II. Applicable materials cross-sections and reactor physics characterization

III. Five Neutronic performance parameters

IV. Breeding capability and core size estimate

V. Self-sustaining breeding in (breed and burn) open cycle

VI. Burnup definition for liquid fuel

VII. Radionuclides distribution and release during accidental conditions

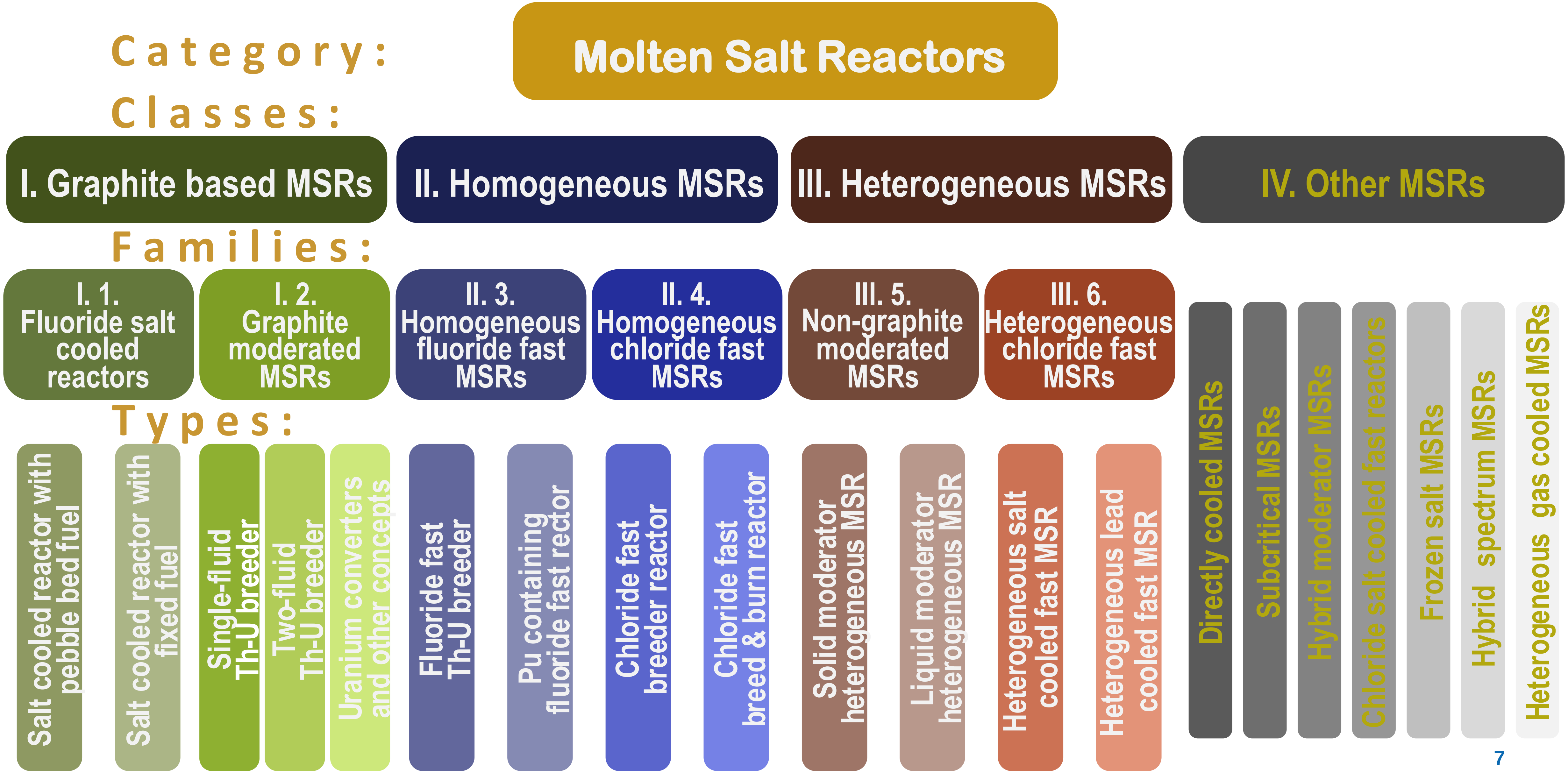
Definition of MSRs:

MSR is any reactor where a molten salt has a prominent role in the reactor core (i.e., fuel, coolant, and/or moderator).

IAEA Technical Report Series, Status of Molten Salt Reactor Technology, document in preparation, International Atomic Energy Agency, 2021.

MSR taxonomy

Taxonomy



Adopted from: IAEA Technical Report Series, Status of Molten Salt Reactor Technology, document in preparation, International Atomic Energy Agency, 2021.

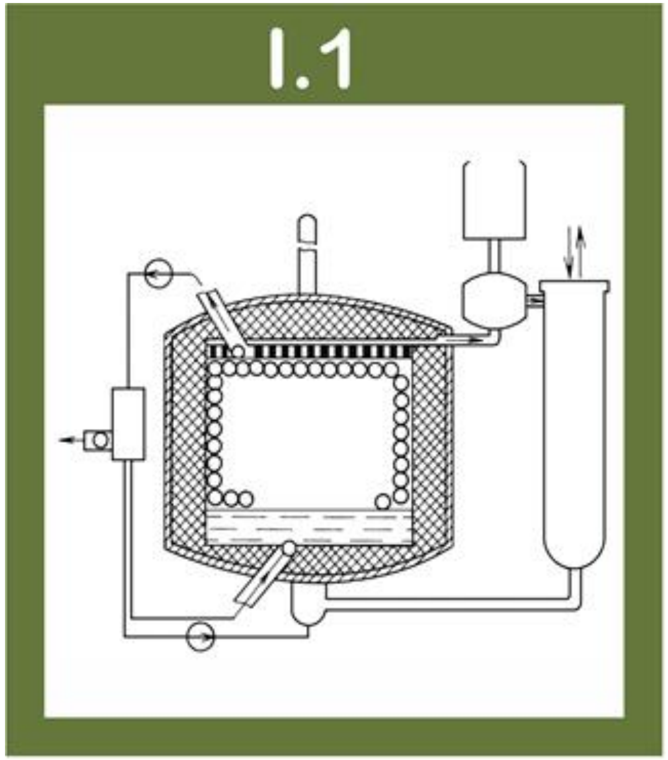
F.I.1. Fluoride salt cooled reactors

Salt cooled reactor with pebble bed fuel

Salt cooled reactor with fixed fuel

Types definition: *By fuel form (pebble bed vs. prismatic or compacts)*
Primary heat exchange: *In core*
Heat convection by fuel: *No, dedicated coolant* ***LiF-BeF$_2$*** *(Li is enriched to ^{7}Li)*
Fuel form: *TRISO-particles in graphite matrix*
Struct. material in core: *No, graphite moderator and coolant salt are compatible*
Neutronic performance: *Converter*
Self-sustaining breeding: *Cannot be achieved*
Major fuel cycle: *Enr. U converter*
Leakage utilization: *Reflector*
Characteristic:

- ***^{7}LiF-BeF$_2$*** *has certain moderation power, hence it has* ***negative density effect*** *on reactivity.*
- *Very low specific fuel density in some designs:*
  - → *Unprocessed* ***spent fuel is volumetric****.*
  - → *Increased non-fuel parasitic neutron captures.*
  - → *Core transparency for neutrons (neutron leakage).*



*BELOUSOV, I.G., et al., Features layout of VTRS for technological purpose, VANTS 16 3 (**1983**) 13–14*

Single-fluid Th-U breeder

Two-fluid Th-U breeder

Uranium converters and other concepts

F.I.2. Graphite moderated MSRs

Types definition: *By fuel cycle type (Th-U breeder or enr. U converter)*

Primary heat exchange: *Ex core*

Heat convection by fuel: *Yes*

Fuel form: *Ac. diluted in fluorides salts, for breeders it is exclusively* ***^{7}LiF-BeF$_2$*** *(^{7}LiF?)*

Struct. material in core: *No, graphite moderator and coolant salt are compatible*

Neutronic performance: *Breeder or converter*

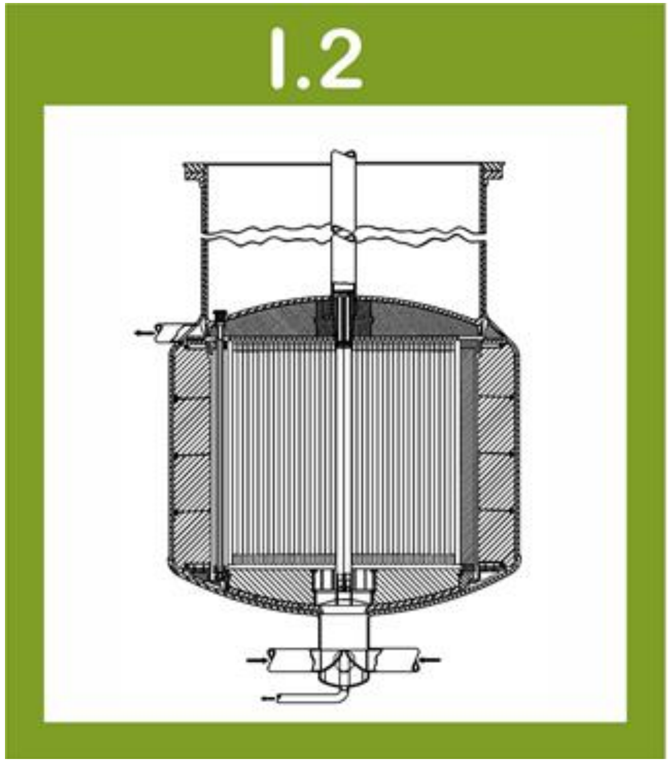
Self-sustaining breeding: *Can be achieved, is demanding*

Major fuel cycle: *Closed Th-U or enr. U converter*

Leakage utilization: *Reflector, multi-zone core, blanket*

Characteristic:

- *Specific fuel density is higher than in Fluoride salt cooled reactors.*
- *Limited graphite life-span as the only reason for its exchange.*
- *Hastelloy vessel protected by graphite reflector.*
- *Need of fast FPs removal and/or ^{233}Pa separation to achieve self-sustaining breeding.*



R. C. Robertson, Conceptual Design Study of a Single-Fluid Molten-Salt Breeder Reactor. ORNL-4541, ***(1971)***

F.II.3. Homogeneous fluoride fast MSRs

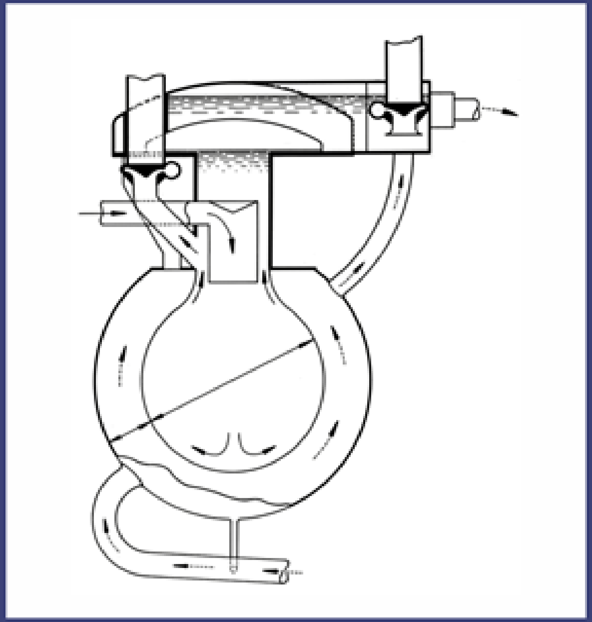
Fluoride fast Th-U breeder

Pu containing fluoride fast rector

Types definition: *By fuel cycle type (Th-U breeder, enr. U converter, burner)*
Primary heat exchange: *Ex core*
Heat convection by fuel: *Yes*
Fuel form: *Ac. diluted in fluorides salts, for breeders it is typically* ***^{7}LiF*** *(FLiNa, FNaK?)*
Struct. material in core: *No, homogeneous salt-filled core*
Neutronic performance: *Breeder, converter, dedicated burner*
Self-sustaining breeding: *Can be achieved*
Major fuel cycle: *Closed Th-U (U-Pu), enr. U conv., burner*
Leakage utilization: *Blanket, Reflector (Hastelloy)*
Characteristic:

- *Hastelloy vessel is exposed to neutron flux and should be regularly replaced.*
- *Moderation power of ^{7}LiF:*
  - → *Softest fast spectra.*
  - → *Low transparency for neutrons.*
  - → *Possibility of compact cores.*

II.3



*MACPHERSON, H. G., Rep. ORNL-2474, Oak Ridge Natl Lab., TN (**1958**)*

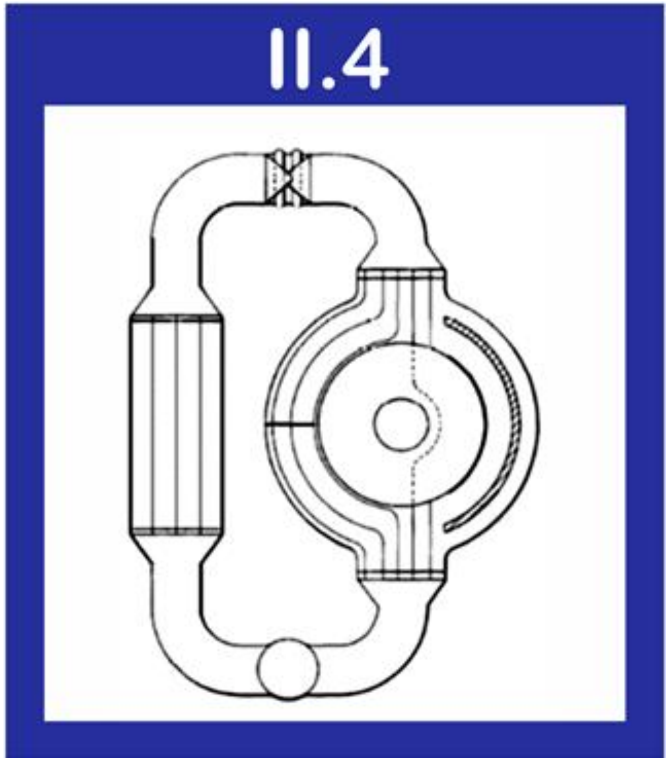
F.II.4. Homogeneous chloride fast MSRs

Chloride fast breeder reactor

Chloride fast breed & burn reactor

Types definition: *By fuel cycle type (U-Pu breeder or breed & burn cycle)*
Primary heat exchange: *Ex core*
Heat convection by fuel: *Yes*
Fuel form: *Ac. diluted in chloride salts, for breeders it is typically* ***$Na^{37}Cl$***
Struct. material in core: *No, homogeneous salt-filled core*
Neutronic performance: *Breeder, Breed and Burn*
Self-sustaining breeding: *Can be achieved*
Major fuel cycle: *Closed U-Pu or Breed-and-Burn U-Pu*
Leakage utilization: *Blanket, Reflector (lead?)*
Characteristic:

- *Reactor vessel is exposed to neutron flux and should be regularly replaced.*
- *Absence of scattering / moderation power:*
  - → *Transparent for neutrons.*
  - → *Hardest spectra from all fast reactors.*
  - → *Large reactor cores, unsuitable for Th-U cycle.*



*Bulmer J, et al., Fused Salt Fast Breeder. ORNL, CF-56-8-204, (**1956**)*

F.III.5. Non-graphite moderated MSRs

Solid moderator heterogeneous MSR

Liquid moderator heterogeneous MSR

Types definition: *By moderator state (solid or liquid moderator)*

Primary heat exchange: *Ex core**

Heat convection by fuel: *Yes**

Fuel form: *Ac. diluted in fluorides salts, for breeders it is exclusively ^{7}LiF-BeF_2 (^{7}LiF?)*

Struct. material in core: *Yes, for separation of fuel salt and moderator*

Neutronic performance: *Converter, burner*

Self-sustaining breeding: *Impossible or very demanding***

Major fuel cycle: *Closed Th-U**, enr. U converter, burner*

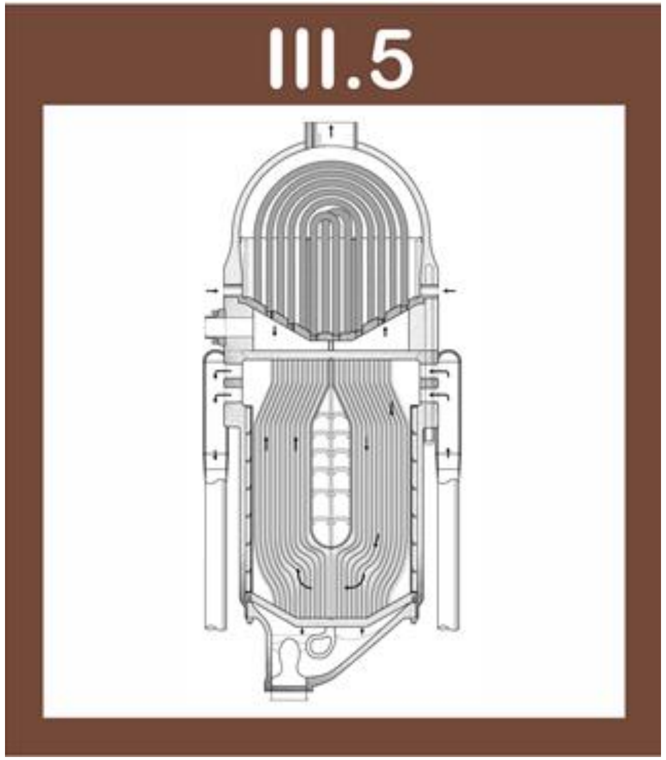
Leakage utilization: *Reflector (moderator)*

Characteristic:

- *Moderator requires structural material for separation:*
  - → *Limited life-span of separation material.*
  - → *Determination of neutronic performance.*

* *Unless if liquid moderator acts as coolant.*

** *Relying on low capture structural material (SiC, C composites?).*



FRAAS, A.P., SAVOLAINEN, A.W., Rep. ORNL-1721, Oak Ridge Natl Lab., TN (**1954**)

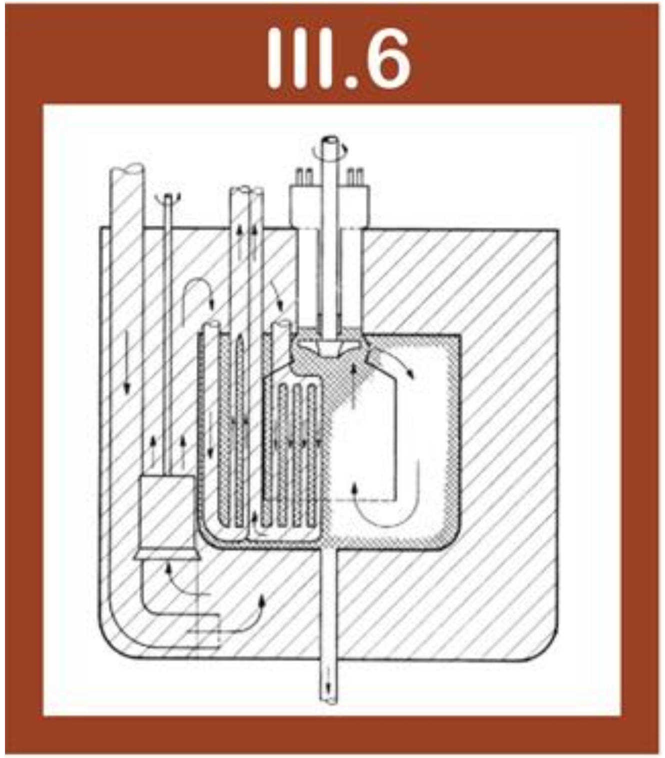
F.III.6. Heterogeneous chloride fast MSRs

Heterogeneous salt cooled fast MSR

Heterogeneous lead cooled fast MSR

Types definition: *By dedicated coolant type (salt or lead cooled)*
Primary heat exchange: *In core*
Heat convection by fuel: *Usually no, dedicated coolant*
Fuel form: *Ac. diluted in chloride salts, for breeders it is typically* $\boldsymbol{Na^{37}Cl}$
Struct. material in core: *Yes, for separation of fuel salt and dedicated coolant*
Neutronic performance: *Converter, Breeder, B&B is demanding*
Self-sustaining breeding: *Can be achieved*
Major fuel cycle: *Closed U-Pu or enr. U converter*
Leakage utilization: *Blanket, Reflector (lead?)*
Characteristic:

- *Coolant requires structural material for separation:*
  - → *Limited life-span of separation material.*
  - → *Reduced neutronic performance.*
  - → *It provides additional scattering XS.*
  - → *Possibly smaller cores that homogeneous chloride fast MSRs.*



*Taube M and Ligou J, Report EIR-215 Wurenlingen, Switzerland (**1972**).*

Applicable materials cross-sections

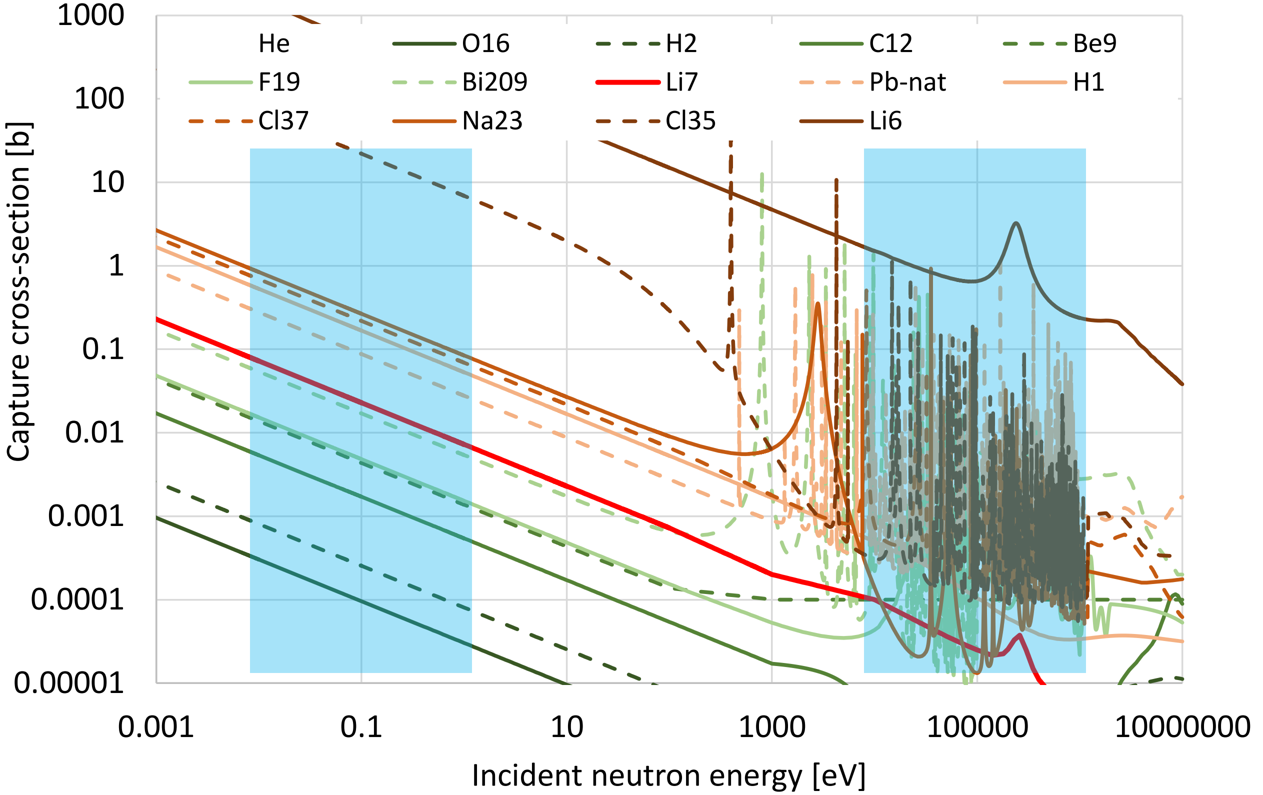
Overview of applicable materials

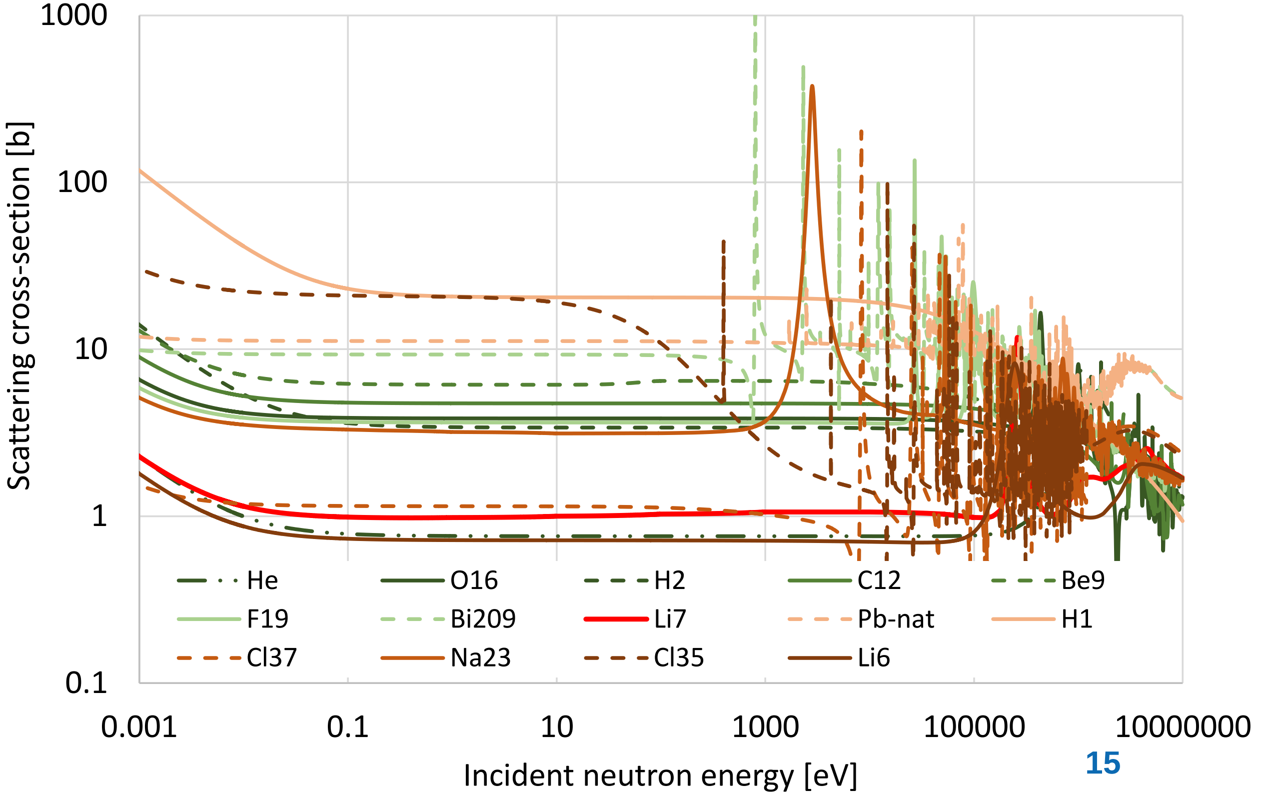
Water (light & heavy): ^{1}H, ^{2}H, ^{16}O
Liquid metals (sodium, lead, lead-bismuth): ^{23}Na, ^{nat}Pb, ^{209}Bi
Gases (helium, CO_2): ^{4}He, ^{12}C, ^{16}O
Salts (fluorides, chlorides): ^{6}Li, ^{7}Li, ^{9}Be, ^{19}F, ^{nat}Mg, ^{35}Cl, ^{37}Cl, ^{nat}K, ^{nat}Ca

BTW:

***Capture XS:** 1/v rule, i.e. capture chance depends on the time, which neutrons and nuclei spend together.*

***Scattering XS** is rather flat and based on "geometrical" interaction.*





Range for averaging around 0.1ev and 0.1MeV.

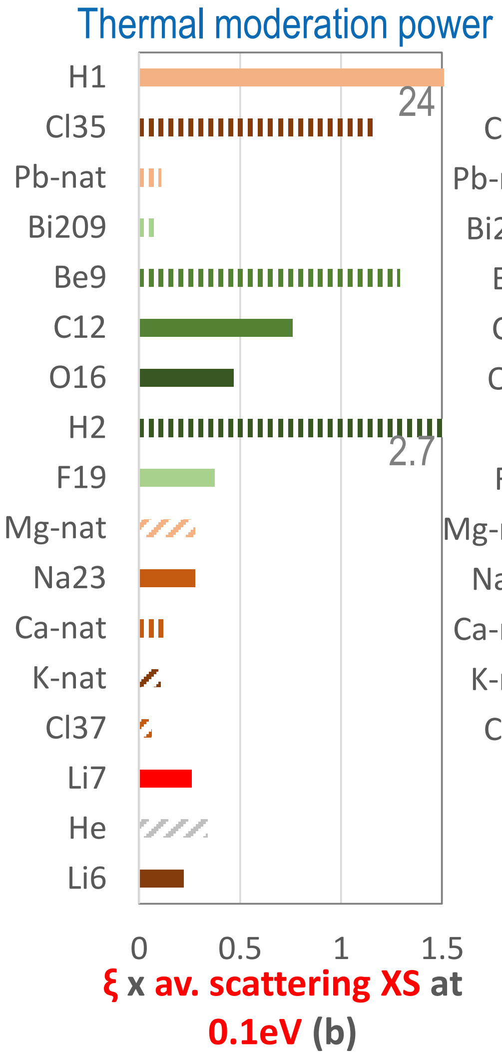
Data from ENDF/B VII.0 library

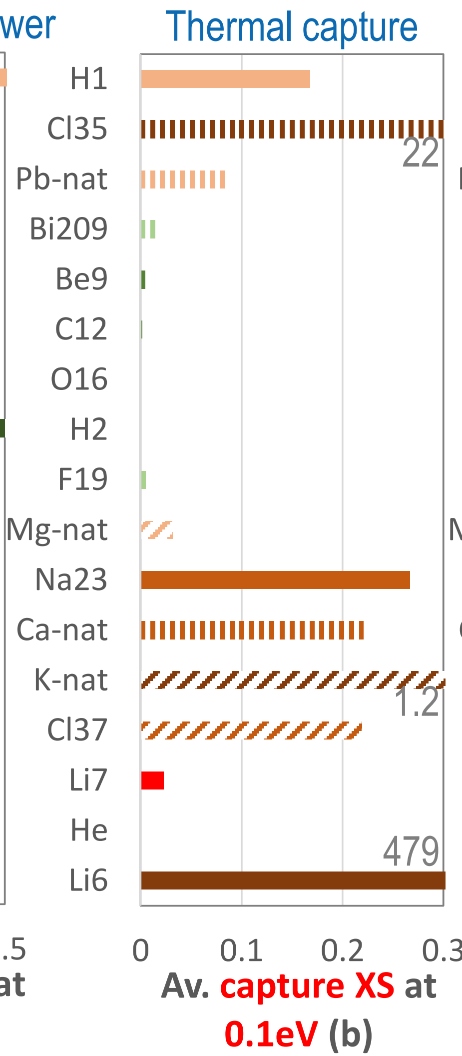
Moderation power and capture XS

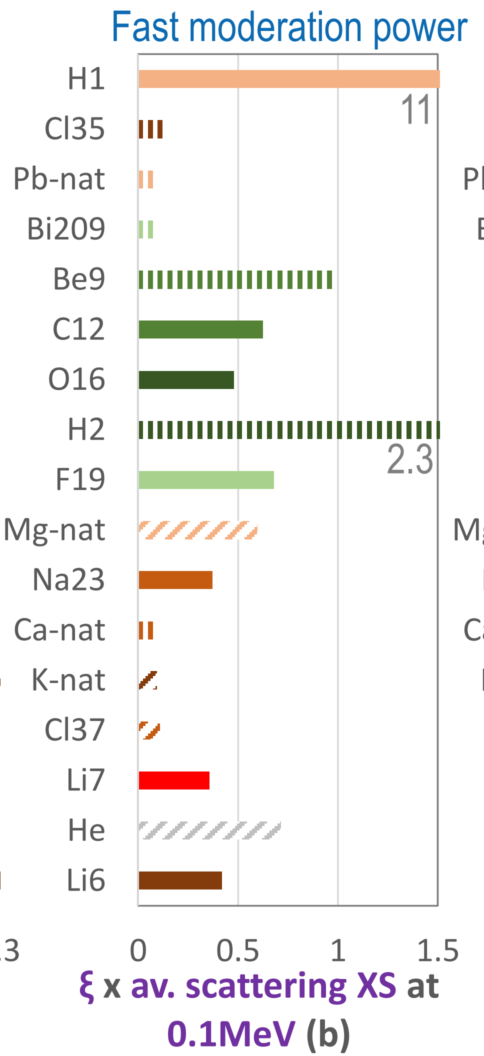
Logarithmic decrement of energy *ξ* describes neutron energy loss by scattering.

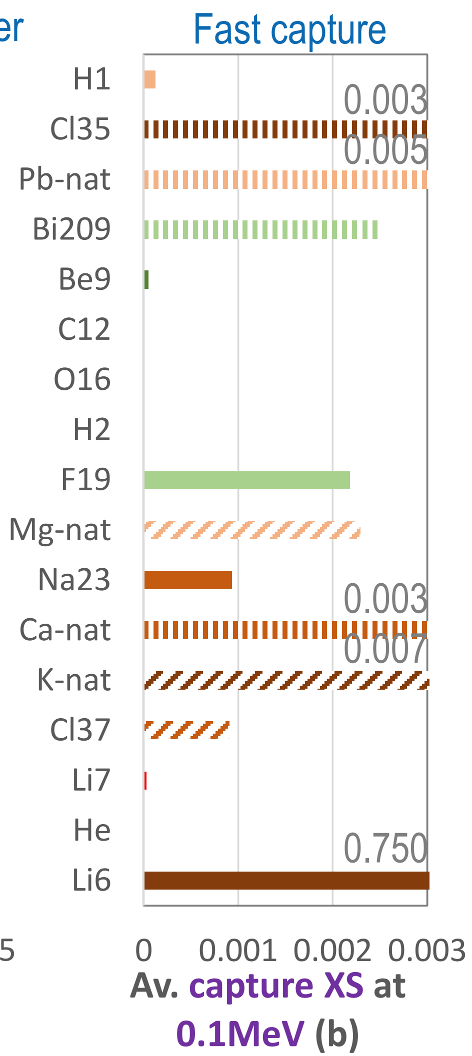
Product of *ξ* and **scattering XS** is used here as a **moderation power*** criteria.

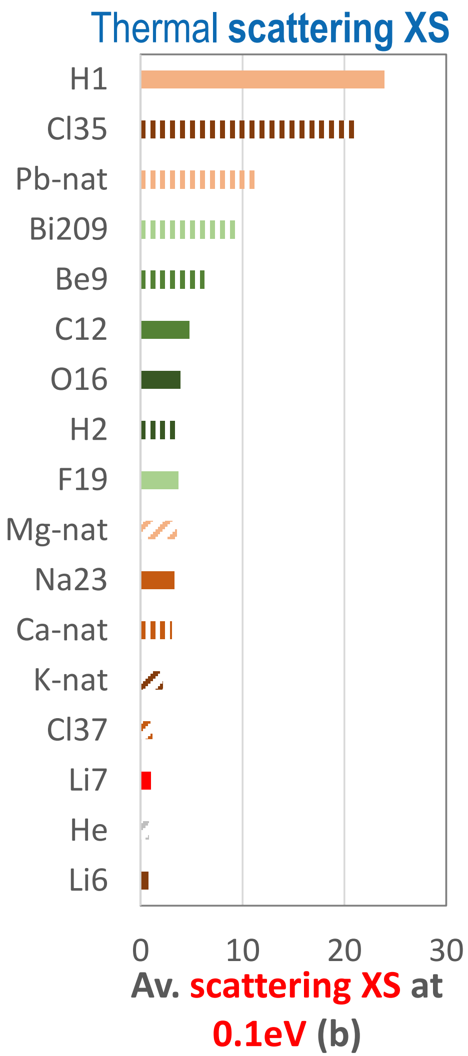
**It is not a standard definition, because it uses microscopic instead of macroscopic XS.*









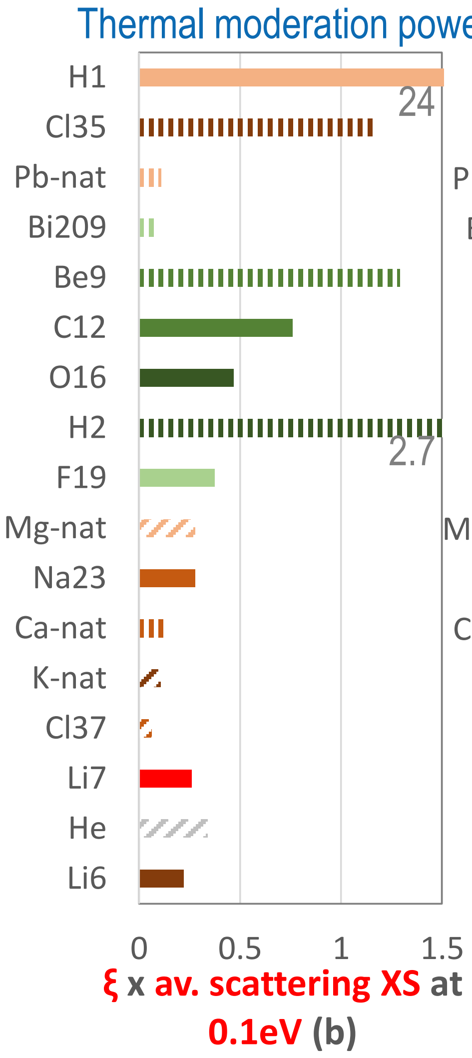


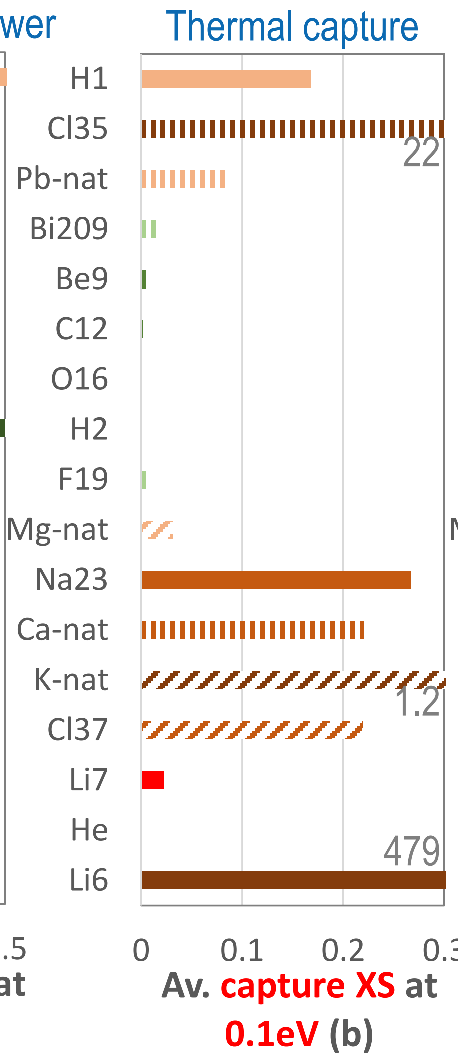
x

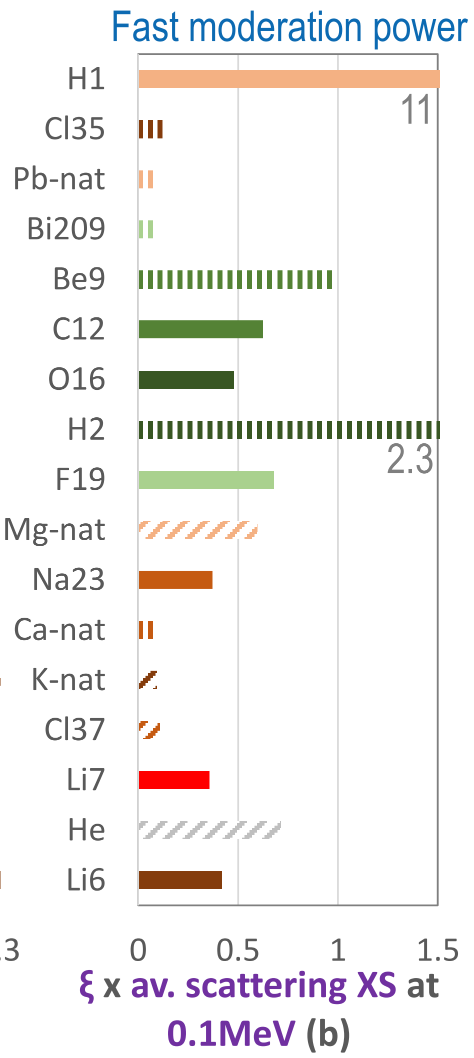
ξ
1.000
0.056
0.010
0.010
0.207
0.158
0.120
0.725
0.102
0.078
0.084
0.045
0.049
0.053
0.260
0.425
0.299

Summary of materials characteristics

Based on the moderation power and capture XS, 4 coolant nuclides performance characteristics can be defined:







	Moderator:	Suppressing fast neutrons:	Breeding in thermal spectrum:	Breeding in fast spectrum:
H1	Yes*	Yes	No	No
Cl35	No	No	No	No
Pb-nat	No	No	No	Yes
Bi209	No	No	No	Yes
Be9	Yes	Yes	Yes	No
C12	Yes	Yes	Yes	No
O16	No	No	Yes	Yes
H2	Yes	Yes	Yes	No
F19	No	Yes**	Yes	Yes***
Mg-nat	No	Yes**	Yes	Yes
Na23	No	No	No	Yes
Ca-nat	No	No	No	Yes
K-nat	No	No	No	Yes
Cl37	No	No	No	Yes
Li7	No	Yes**	Yes	Yes
He4	No	No	Yes	Yes
Li6	No	Yes**	No	No

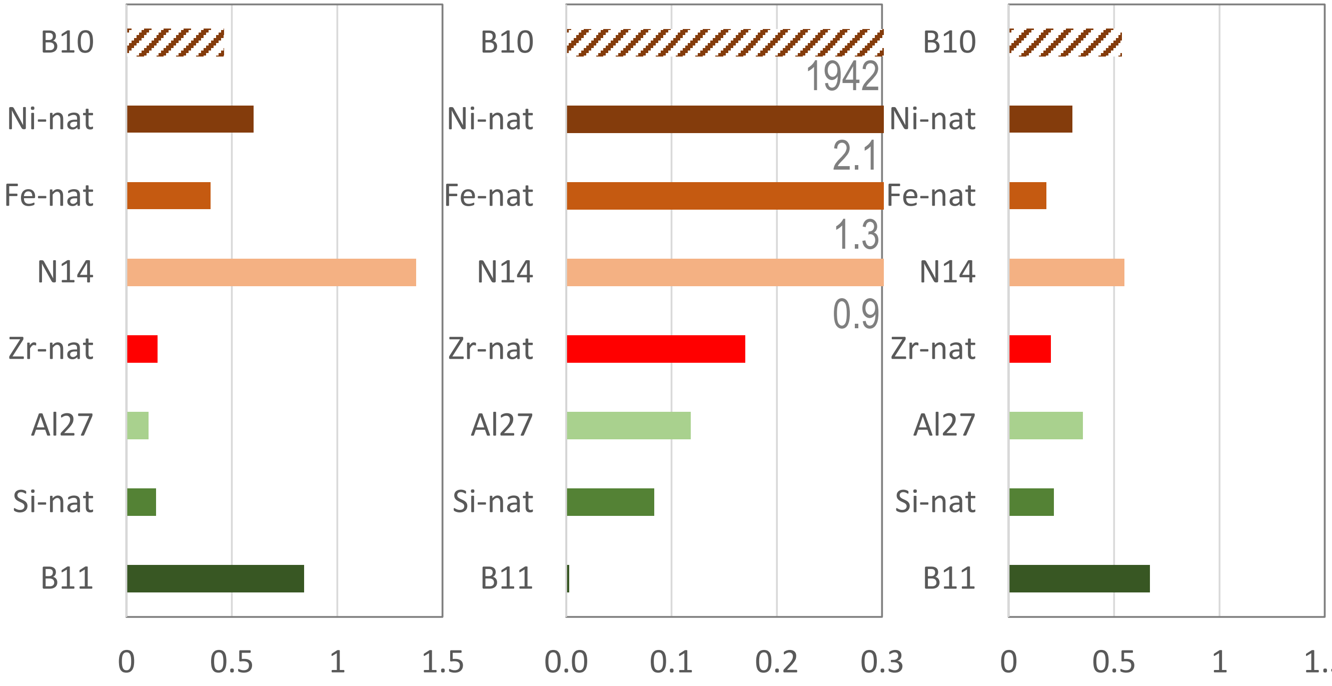
*Substantial capture XS

**Broad Scattering resonances around 0.1MeV

***However the spectrum is quite soft.

Performance of structural materials

Boron (^{10}B, ^{11}B) as a absorber,
^{14}N as ^{16}O alternative.
Si as part of SiC,
Aluminum, **Zirconium**, **Iron** and **Nickel**.



ξ x av. scattering XS at 0.1eV (b)

Av. capture XS at 0.1eV (b)

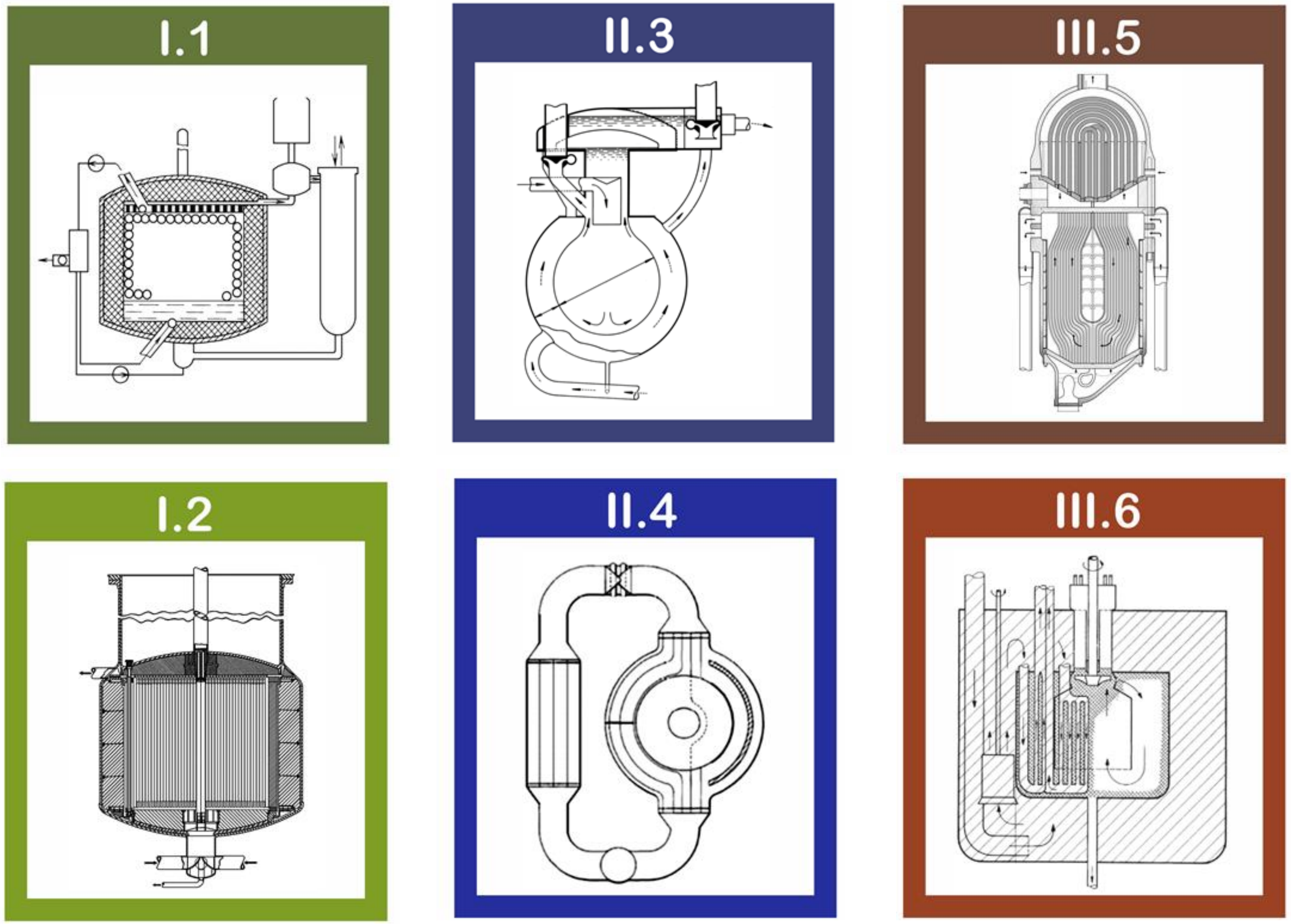
ξ x av. scattering XS at 0.1MeV (b)

- **Zirconium:** similar capture XS as ^{1}H.
- **Silicon:** similar capture XS as lead. *(big hope for many MSR concepts)*
- **Aluminum:** sometimes used as metallic fuel matrix for research reactors.
- **Iron (steel)** can be used in fast reactors but should be avoided in thermal spectrum.
- **Nickel (alloys)** foreseen for MSRs because of chemical resistance have **2x higher capture XS** than iron.
- Presence in the core, as a fuel cladding:
  1) Should be avoided in thermal systems.
  2) Reduce performance of fast systems.

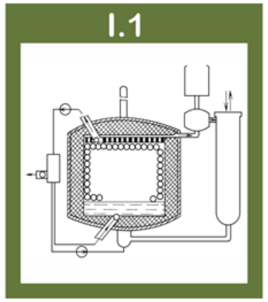
Characterization
from
reactor physics perspective

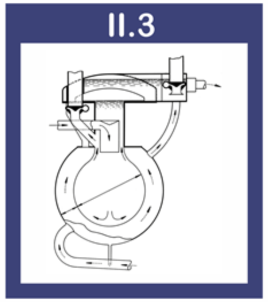
Six major MSR families

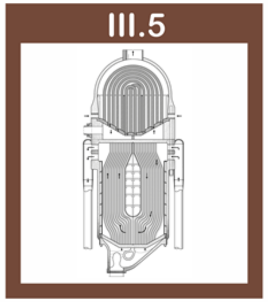
- **I.1.** Fluoride salt cooled reactors
- **I.2.** Graphite moderated MSRs
- **II.3.** Homogeneous fluoride fast MSRs
- **II.4.** Homogeneous chloride fast MSRs
- **III.5.** Non-graphite moderated MSRs
- **III.6.** Heterogeneous chloride fast MSRs



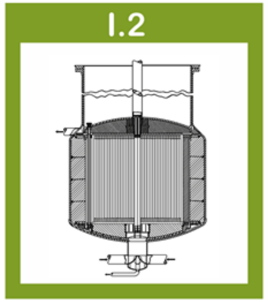
Reactor physics features / issues

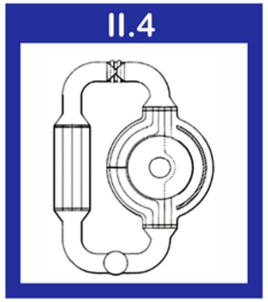


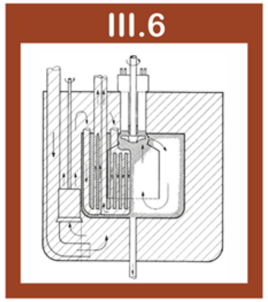




• Double heterogeneity	(I.1)
• Graphite limited lifespan and positive temperature effect	(I.2)
• Positive coolant and blanket density effect	(I.1, III.5, III.6)
• Large migration area	(I.1, I.2, II.4, partly III.6)
• Fuel volumetric heat up and homogenization	(I.2, II.3, II.4, partly III.5, III.6)
• Power level and peaking in core	(I.1, partly III.5, III.6)
• Local overheating or excessive burnup	(I.2, II.3, II.4, partly III.5, III.6)
• Fission Products (FPs) circulation	(I.2, II.3, II.4, optionally III.5, III.6)
• Gaseous and non-soluble FPs removal	(I.2, II.3, II.4, III.5, III.6)
• ^{233}Pa longer half-life than ^{239}Np	(all when operated in Th-U cycle)
• Limited structural material lifespan	(all families)







Krepel J., Ragusa C., MSR Reactor physics: characterization, neutronic performance, multiphysics coupling, and reduced-order modeling, chapter 4 ,Vol. 1 of a book: Dolan, T., J., Molten Salt Reactors and Thorium Energy, 2nd Edition, in preparation.

Neutronic performance parameters

Five fuel cycle performance parameters

I. Breeding capability

- How many neutrons can be captured by ^{232}Th or ^{238}U so that the reactor is still critical.
- BTW: Uranium enrichment reduces ^{238}U capture, hence also the breeding capability.
- It is about neutron economy.

II. Achievable burnup

- Is limited by FPs neutron capture and by fuel irradiation stability.
- Depends on initial reserve of fissile material and its renewal (breeding capability).

III. Initial fissile mass

- It is determined by neutron economy and spectrum type of the reactor.
- Higher burnup may impose higher initial fissile mass reserve.

IV. Means of criticality maintenance

- Ac. irradiation and FPs creation results in reactivity oscillations / swing.
- Compensation option for reactivity swing differ between reactor types.

V. Transmutation capability

- “Neutron costs” and “speed” of synthetic actinides fission.
- Synthetic Ac. compatibility with the fuel and fabrication process.

MSR: possible absence of structural materials

Radiation stability of the salt

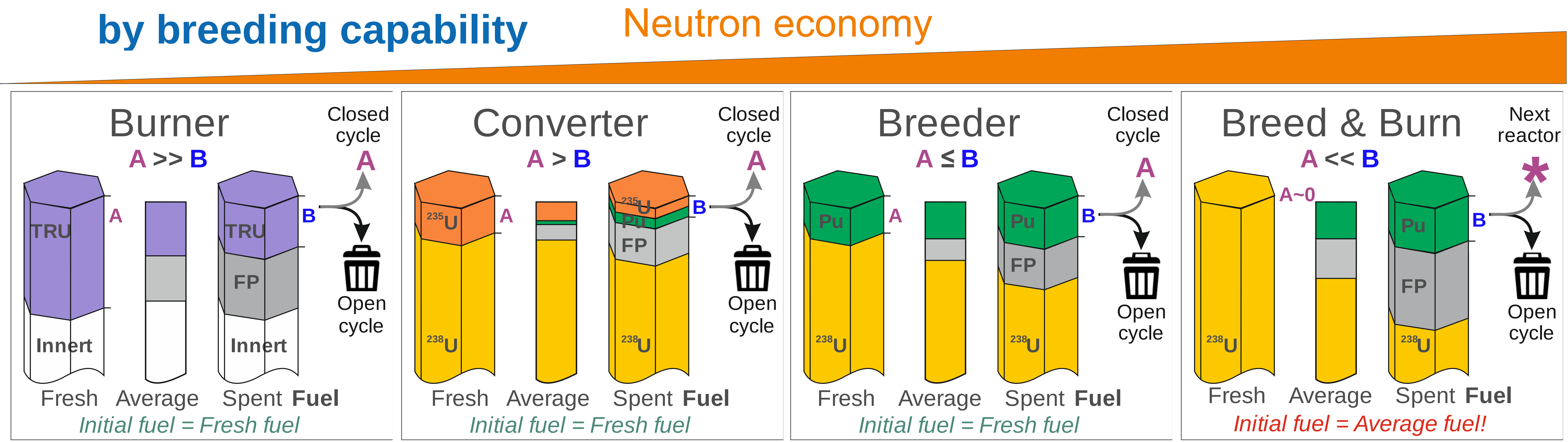
Online refuelling and removal of some FPs

Possible liquid fuel reshaping / draining

Absence of fabrication
Solubility of actinides?

Krepel, J., Self-sustaining breeding in advanced reactors: Comparison of fuel cycle performance, Encyclopedia of Nuclear Energy, (Greenspan, E., Ed.), Elsevier, 2021.

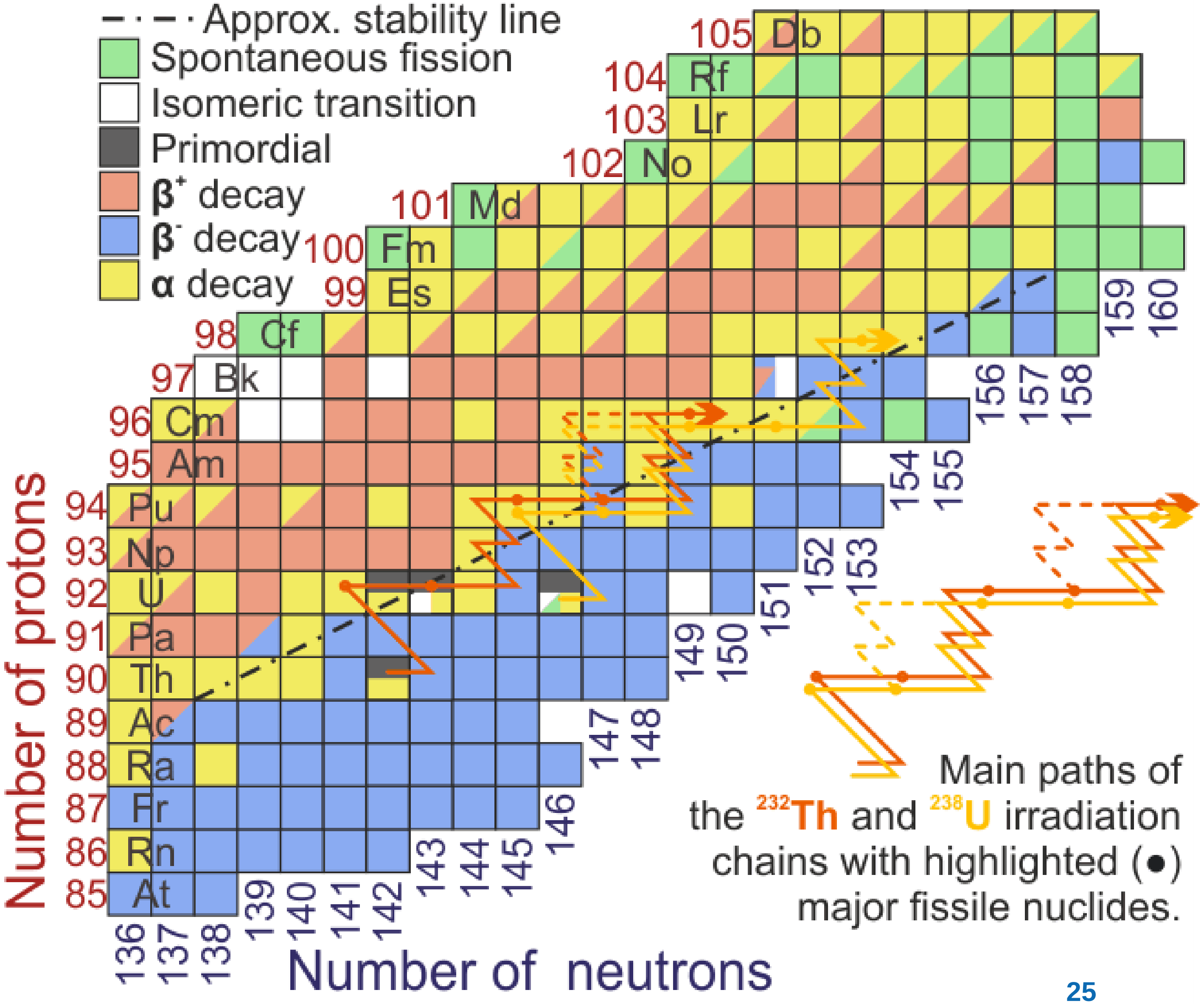
Reactor classification by breeding capability



- Burner typically relies on synthetic Actinides (Ac) and excludes fertile isotopes as ^{238}U or ^{232}Th.
- Convertor, e. g. PWR or DMSR, is usually operates in open fuel cycle and burns ^{235}U.
- Breeder profit from neutronics advantages only in the closed cycle.
  For Iso-breeding (EU) or Break-even (US) reactor => A=B.
- Extreme breeder can be operated in Breed & Burn mode.
  It can have high fuel utilization even without reprocessing.

Major path of the ^{232}Th and ^{238}U irradiation chains

- ^{232}Th and ^{238}U irradiation chains are similar, because of the repetitiveness of actinides properties (+2p +4n).
- Nonetheless, there is the exception caused by ^{241}Pu fast decay (x^{235}U).
- Furthermore, nuclides in ^{238}U chain have more nucleons and generally slightly **shorter half-lives**.
- For the same reason, they produce **more neutrons** per fission.



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Krepel, J., Self-sustaining breeding in advanced reactors: Characterization of natural resources, Encyclopedia of Nuclear Energy, (Greenspan, E., Ed.), Elsevier, 2020.

Neutron balance of the equilibrium actinide chains

- The major indicator for **breeding capability** is the **neutron balance**.
- It has several **components**: neutron leakage, neutron parasitical absorption on non-actinides materials and **neutron balance of actinides itself**.
- Neutron balance of the equilibrium actinides composition can be enumerated by:

1. Eta-2 with correction factors:

$$Balance_1 = \eta_{233U} - 2 + F_{232Th} - \frac{C_{233U}}{C_{233U} + F_{233U}} D_{234U} - \left(2 \frac{C_{233Pa}}{C_{233U} + F_{233U}} + \frac{C_{233Pa}}{C_{233U} + F_{233U}} D_{234U} \right)$$

2. Nu_bar-2 with correction factors:

$$Balance_2 = \bar{\nu} - 2 + F_{232Th} - \frac{\sum_i C_i}{\sum_i F_i} + 2R_{232Th}^{(n,2n)}$$

3. Neutron costs of fission:

$$Balance_3 = \bar{\nu} - \sum_i F_i \left(u_i - 232 + 1 \right) - 4 \sum_i \alpha_i$$

4. D-factor of major fertile nuclide:

$$Balance_4 = -D_{232Th}$$

Neutron balance of the ^{232}Th actinides chain

$$Balance_1 = \eta_{233U} - 2 + F_{232Th} - \frac{C_{233U}}{C_{233U} + F_{233U}} D_{234U} - \left(2\frac{C_{233Pa}}{C_{233U} + F_{233U}} + \frac{C_{233Pa}}{C_{233U} + F_{233U}} D_{234U} \right)$$

$$Balance_2 = \bar{\nu} - 2 + F_{232Th} - \frac{\sum_i C_i}{\sum_i F_i} + 2R_{232Th}^{(n,2n)}$$

$$Balance_3 = \bar{\nu} - \sum_i F_i \left(u_i - 232 + 1\right) - 4\sum_i \alpha_i$$

$$Balance_4 = -D_{232Th}$$

Reactor family	I.1	I.2	I.2	II.3	II.3	II.4	II.4
Reactor type	FHR	MSBR	MSBR	MSFR	MSFR	MCFR	MCFR
Salt used	FLIBE	FLIBE	FLI	FLIBE	FLI	NaCl	AcCl
Migration area	1020	360	309	194	167	1384	1769
$\bar{\nu}$ average	2.50	2.50	2.50	2.52	2.53	2.53	2.53
$\bar{\nu}_{233U}$	2.50	2.50	2.50	2.51	2.52	2.53	2.54
^{232}Th fission probability (F_{232Th})	0.00	0.00	0.01	0.01	0.01	0.03	0.04
^{233}U fission probability (F_{233U})	0.90	0.89	0.89	0.87	0.87	0.90	0.91
^{233}U capture probability (C_{233U})	0.10	0.11	0.11	0.13	0.13	0.10	0.09
^{232}Th D-factor (D_{232Th})	-0.06	-0.15	-0.12	-0.12	-0.20	-0.37	-0.43
^{234}U D-factor (D_{234U})	0.27	0.32	0.36	0.35	-0.02	-0.75	-0.96
Synthetic actinides rel. capture (C_{Ac})	0.44	0.36	0.39	0.42	0.35	0.19	0.15
Neutron balance from η-2							
η - 2	0.25	0.24	0.22	0.18	0.19	0.28	0.31
+ 1 correction term	0.25	0.24	0.23	0.19	0.21	0.31	0.35
+ 1&2 correction terms	0.22	0.21	0.19	0.14	0.21	0.38	0.44
+ 1&2&3 correction terms	**0.06**	**0.15**	**0.12**	**0.11**	**0.19**	**0.37**	**0.42**
Neutron balance from $\bar{\nu}_{233U}$ - 2							
$\bar{\nu}_{233U}$ - 2	0.50	0.50	0.50	0.52	0.53	0.53	0.53
+ 1 correction term	0.50	0.51	0.51	0.53	0.54	0.56	0.57
+ 1&2 correction terms	0.06	0.14	0.12	0.11	0.19	0.36	0.42
+ 1&2&3 correction terms	**0.06**	**0.15**	**0.12**	**0.12**	**0.20**	**0.38**	**0.44**
Neutron balance from $\bar{\nu}$ - fission cost							
$\bar{\nu}$ - fission cost	0.06	0.15	0.12	0.13	0.21	0.37	0.43
+ 1 correction term	**0.06**	**0.15**	**0.12**	**0.12**	**0.19**	**0.37**	**0.43**
Neutron balance from D-factor							
$-D_{232Th}$	**0.06**	**0.15**	**0.12**	**0.12**	**0.20**	**0.37**	**0.43**

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Neutron balance of the ^{238}U actinides chain

$$Balance_1 = \eta_{233U} - 2 + F_{232Th} - \frac{C_{233U}}{C_{233U}+F_{233U}} D_{234U} - \left(2\frac{C_{233Pa}}{C_{233U}+F_{233U}} + \frac{C_{233Pa}}{C_{233U}+F_{233U}} D_{234U} \right)$$

$$Balance_2 = \bar{\nu} - 2 + F_{232Th} - \frac{\sum_i C_i}{\sum_i F_i} + 2R_{232Th}^{(n,2n)}$$

$$Balance_3 = \bar{\nu} - \sum_i F_i \left(u_i - 232 + 1\right) - 4\sum_i \alpha_i$$

$$Balance_4 = -D_{232Th}$$

Reactor family	**I.1**	**I.2**	**I.2**	**II.3**	**II.3**	**II.4**	**II.4**
Reactor type	FHR	MSBR	MSBR	MSFR	MSFR	MCFR	MCFR
Salt used	FLIBE	FLIBE	FLI	FLIBE	FLI	NaCl	AcCl
Migration area	939	380	305	191	177	1205	1874
$\bar{\nu}$ average	2.96	2.95	2.95	2.95	2.95	2.93	2.92
$\bar{\nu}_{239Pu}$	2.86	2.86	2.86	2.91	2.92	2.94	2.95
^{238}U fission probability (F_{238U})	0.00	0.03	0.04	0.05	0.07	0.11	0.15
^{239}Pu fission probability (F_{239Pu})	0.63	0.63	0.63	0.62	0.66	0.79	0.87
^{239}Pu capture probability (C_{239Pu})	0.37	0.37	0.37	0.38	0.34	0.21	0.13
^{238}U D-factor (D_{238U})	0.26	0.21	0.18	-0.01	-0.24	-0.69	-0.90
^{240}Pu D-factor (D_{240Pu})	0.12	0.15	0.13	-0.32	-0.60	-1.10	-1.37
Synthetic actinides rel. capture (C_{Ac})	1.22	1.19	1.17	1.00	0.79	0.36	0.19
Neutron balance from η-2							
η - 2	-0.15	-0.15	-0.15	-0.17	-0.06	0.33	0.55
+ 1 correction term	-0.14	-0.13	-0.11	-0.12	0.01	0.43	0.70
+ 1&2 correction terms	-0.25	-0.24	-0.21	-0.03	0.20	0.67	0.90
+ 1&2&3 correction terms	**-0.26**	**-0.24**	**-0.22**	**-0.03**	**0.20**	**0.67**	**0.90**
Neutron balance from $\bar{\nu}_{239Pu}$ - 2							
$\bar{\nu}_{239Pu}$ - 2	0.96	0.95	0.95	0.95	0.95	0.93	0.92
+ 1 correction term	0.97	0.98	0.99	0.99	1.02	1.04	1.08
+ 1&2 correction terms	-0.25	-0.22	-0.18	-0.01	0.23	0.68	0.89
+ 1&2&3 correction terms	**-0.25**	**-0.21**	**-0.17**	**0.00**	**0.24**	**0.69**	**0.91**
Neutron balance from $\bar{\nu}$ - fission cost							
$\bar{\nu}$ - fission cost	-0.21	-0.11	-0.08	0.26	0.44	0.75	0.93
+ 1 correction term	**-0.25**	**-0.21**	**-0.18**	**-0.01**	**0.23**	**0.68**	**0.90**
Neutron balance from D-factor							
-D_{238U}	**-0.26**	**-0.21**	**-0.18**	**0.01**	**0.24**	**0.69**	**0.90**

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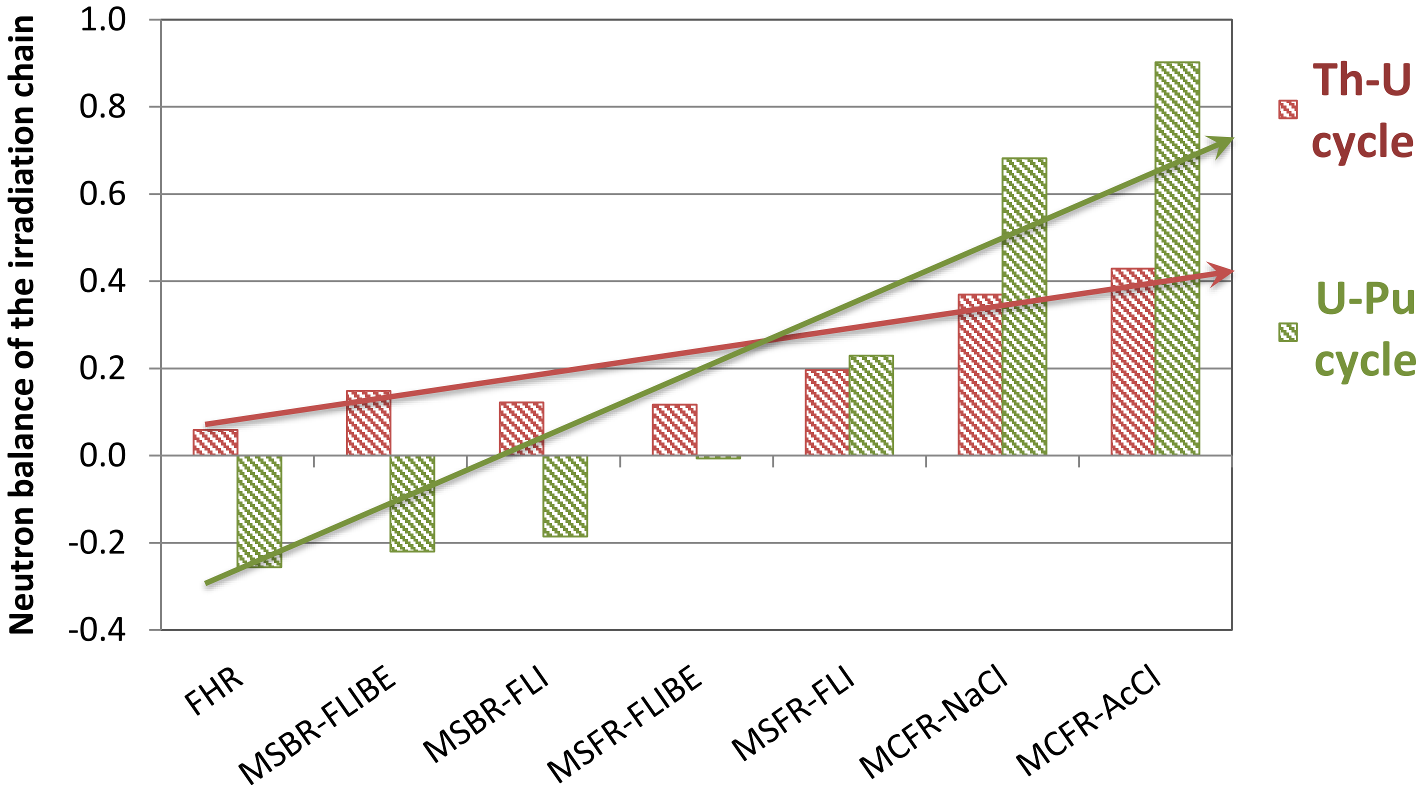
Breeding capability: comparison between ^{232}Th and ^{238}U actinides chain

- ^{238}U actinides chain (U-Pu cycle) profits more from spectrum hardening.
- Better performance:
  Th-U in thermal and
  U-Pu in fast spectra.
- Graphite mod. MSR only in Th-U.
- Fluorides fast MSFR possible in both cycles (almost epithermal).
- Chloride fast MCFR possible in both cycles (bulky core for Th-U).
- B&B possible only for chlorides and U-Pu cycle.



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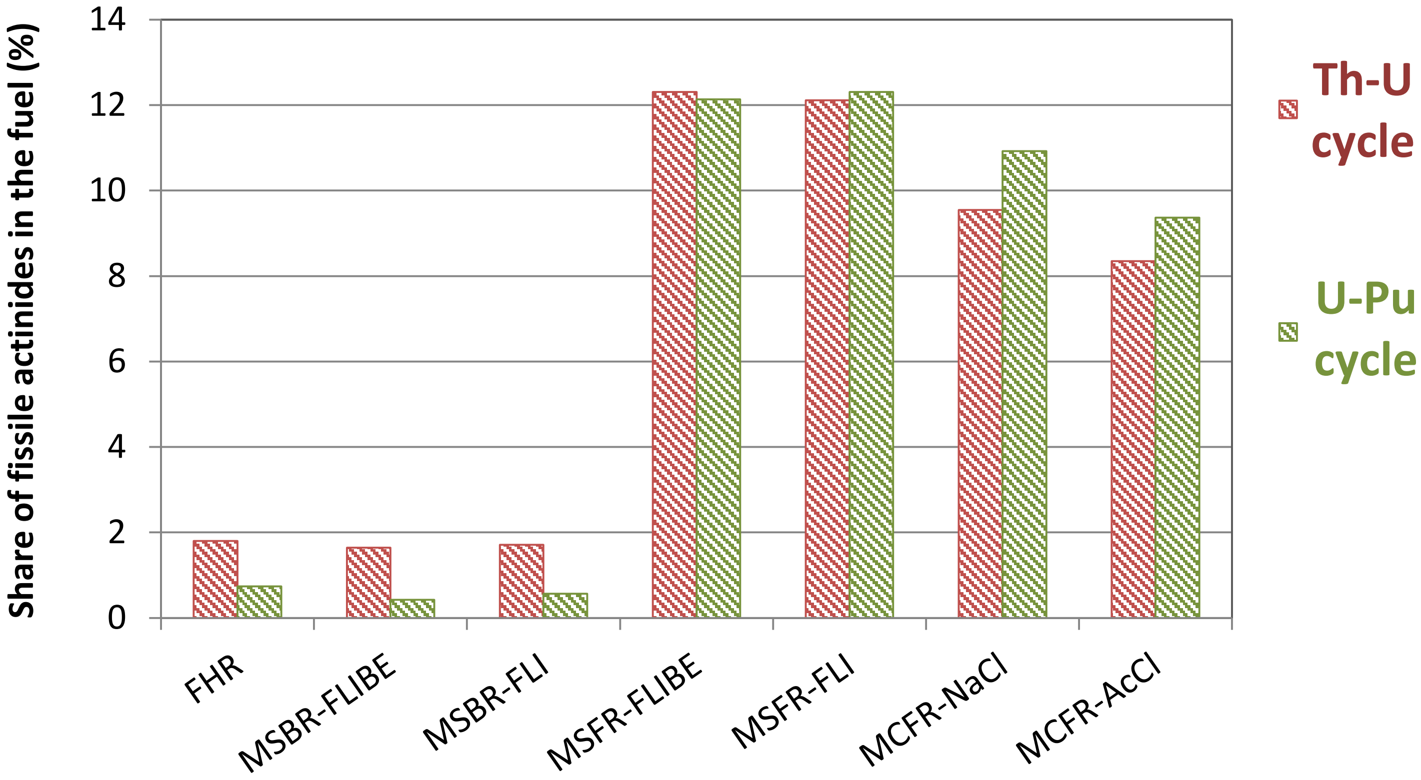
Achievable burnup

- Burnup in liquid fuel will be defined later in this presentation.
- The parasitic neutron captures depends on FPs relative share.
- Fast spectrum reactors have higher fissile actinides share.
- Therefore, they can be operated with higher average FPs share.



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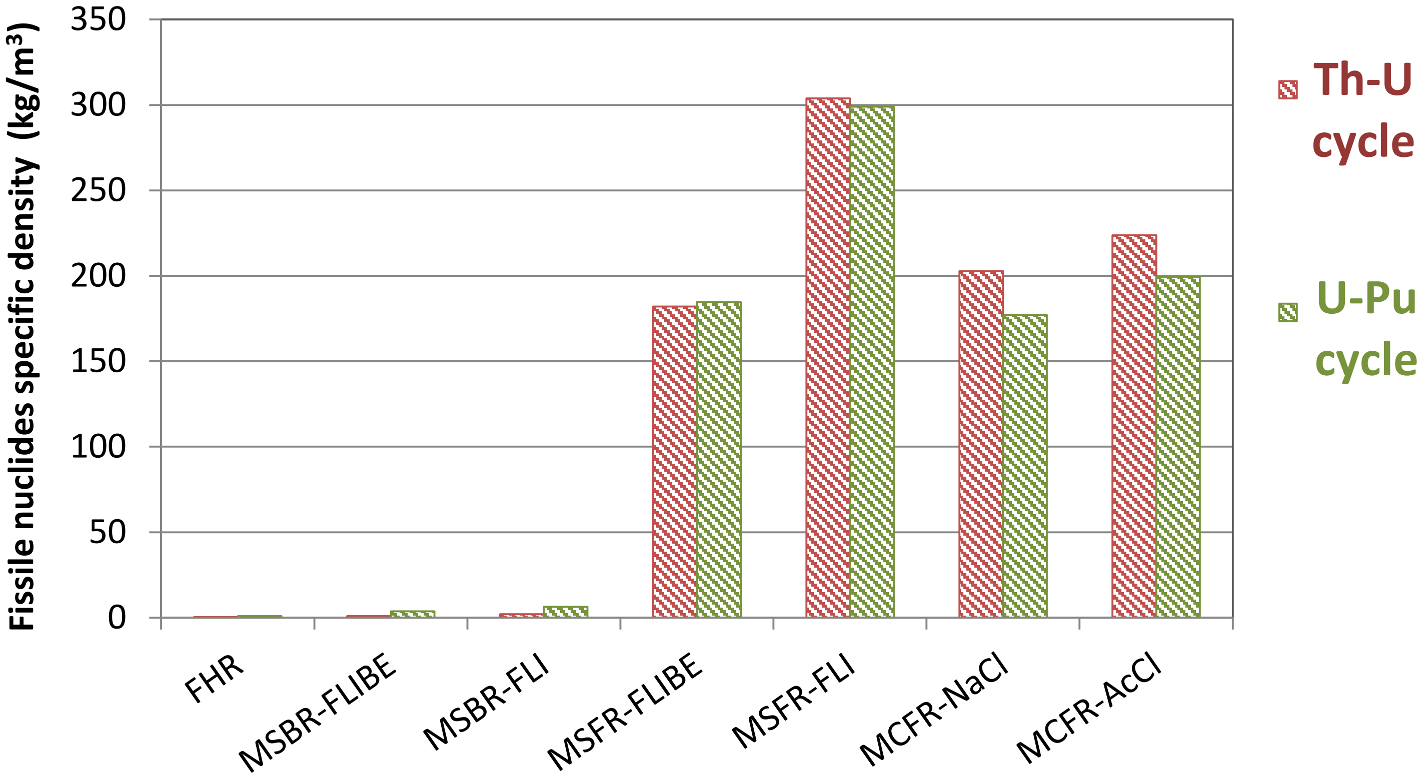
Initial fissile mass

- Initial fissile mass can be defined as a product of core size and fissile actinides specific density.
- In general, initial fissile mass is lower in thermal reactors.
- Especially when moderated by heavy water.



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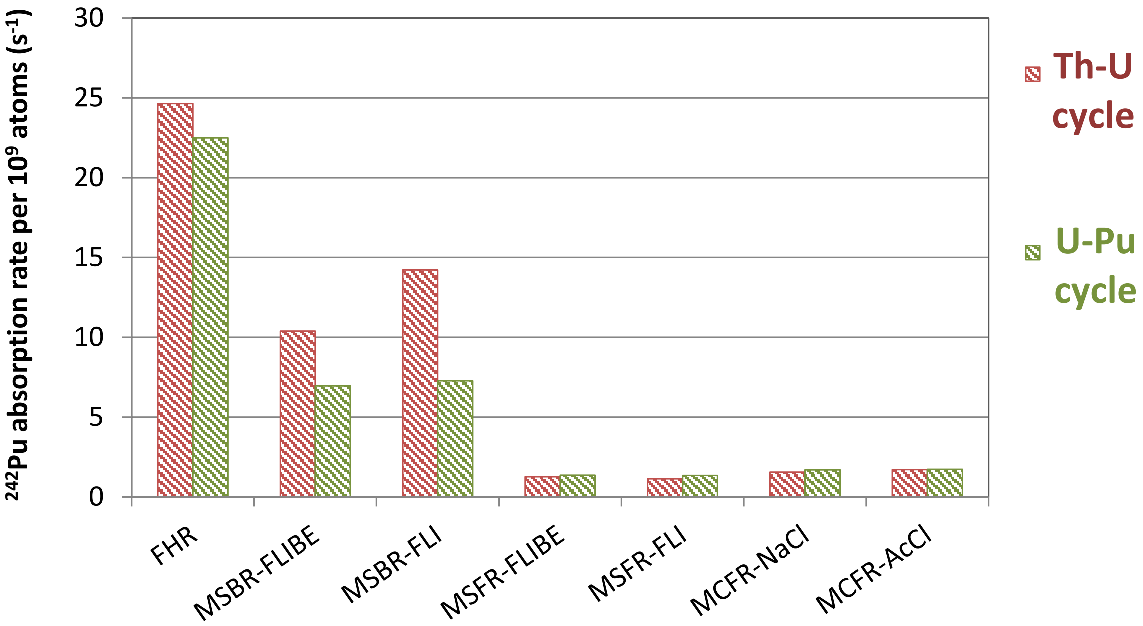
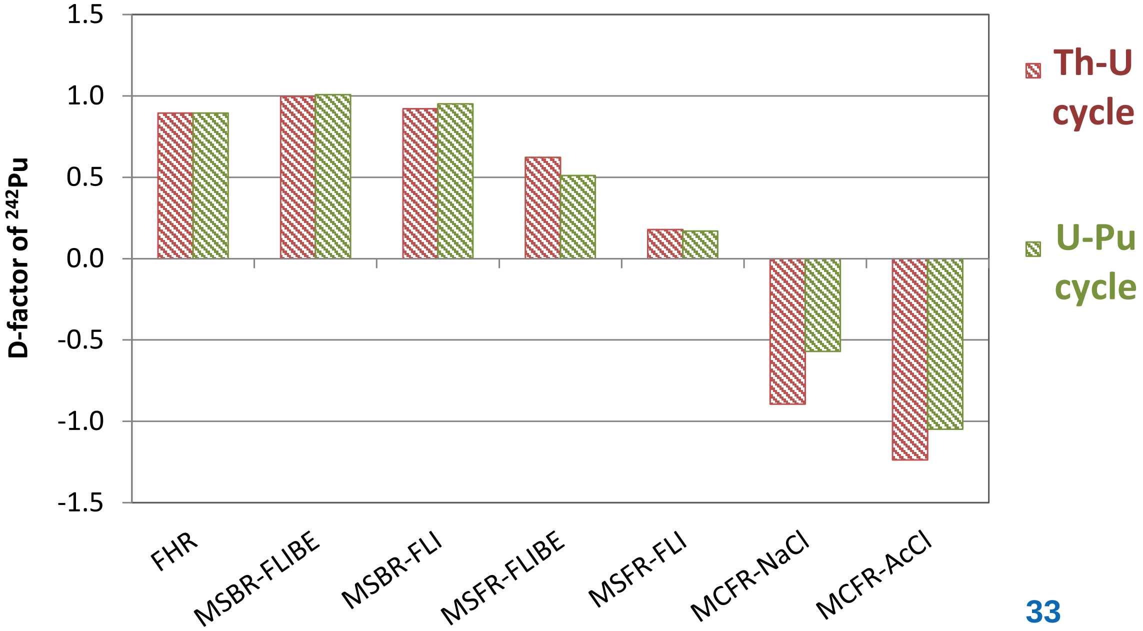
Means of criticality maintenance

- Liquid fuel can allow for online FPs removal and actinides addition.
- It can also allow for unusual reactivity control methods, like salt expelling out of the core.
- For accidental conditions overflow and removal of the respective salt can be used.

Transmutation capability

- In open cycle the increase or decrease of radiotoxicity per produced unit of energy should be considered. (reprocessing losses in closed cycle)
- The "pace" of transmutation per atom is proportional to the respective cross-section.
- The neutron cost of transmutation in closed cycle can be expressed be D-factor. (total neutron cost of given nuclide transmutation together with its daughters)





Breeding capability of moderated MSRs

I.2 family for graphite

III.5 family for other moderators

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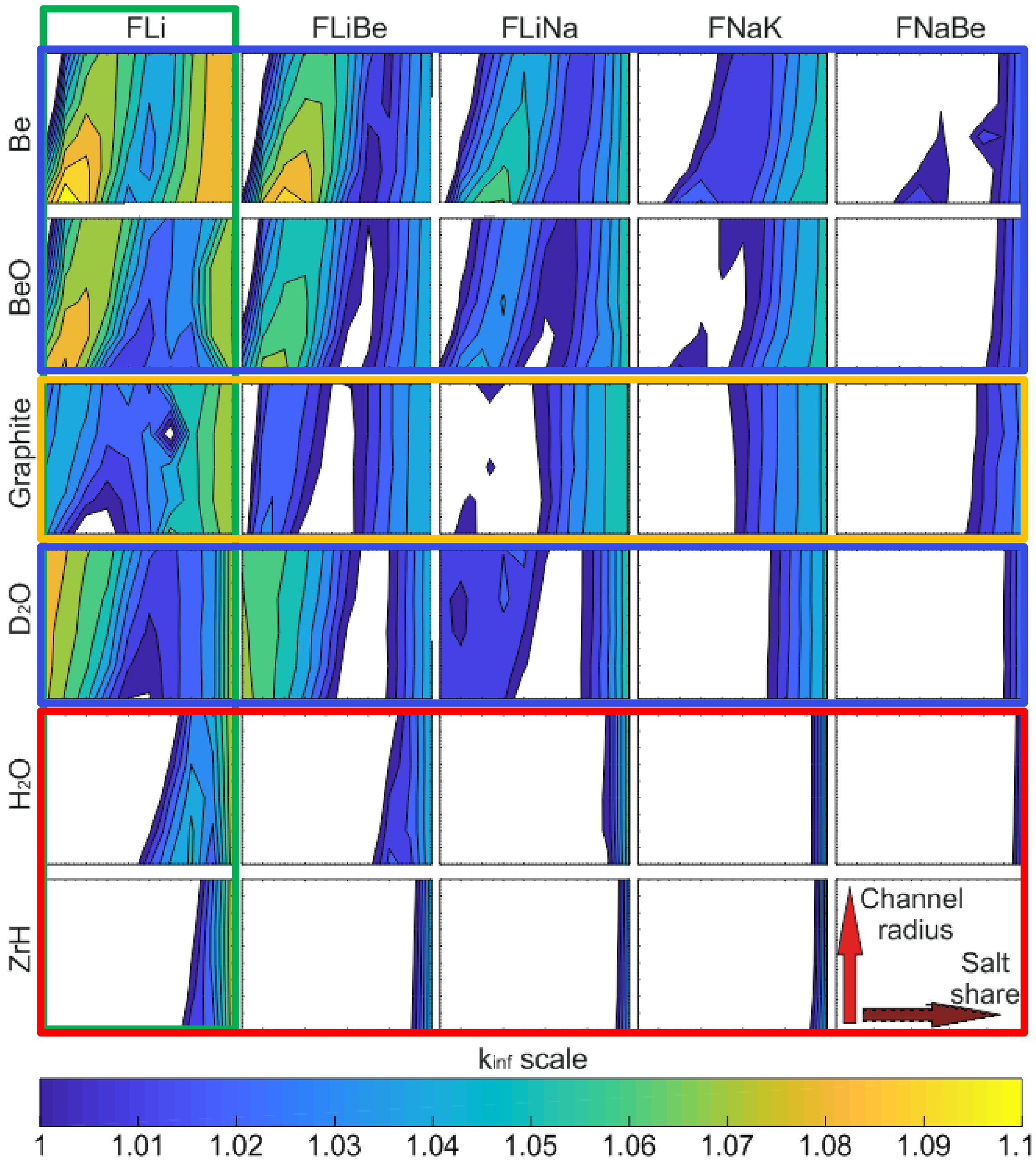
For comparison with other reactors refer to:
Krepel, J., and Losa, E., Self-sustaining breeding in advanced reactors: Characterization of selected reactors, Encyclopedia of Nuclear Energy, (Greenspan, E., Ed.), Elsevier, 2021.

Th-U breeding capability with different moderators

- **5 fluoride salts** were analyzed with **6** selected **moderators**.
- Equilibrium $\boldsymbol{k_{inf}}$ is presented as a function of **salt share** and **channel radius**.
- **FLi** salt is neutronically the best.
- Good results for **Be, BeO, and D_2O**; however, they are not compatible with the salt without cladding (SiC..?).
- Hydrogen based moderators **ZrH and H_2O** not applicable for closed cycle.
- **Graphite** is not the best moderator, but the only one directly compatible with salt.



Hombourger, B.A., 2018. Ph.D. Thesis. EPFL Lausanne, Switzerland.

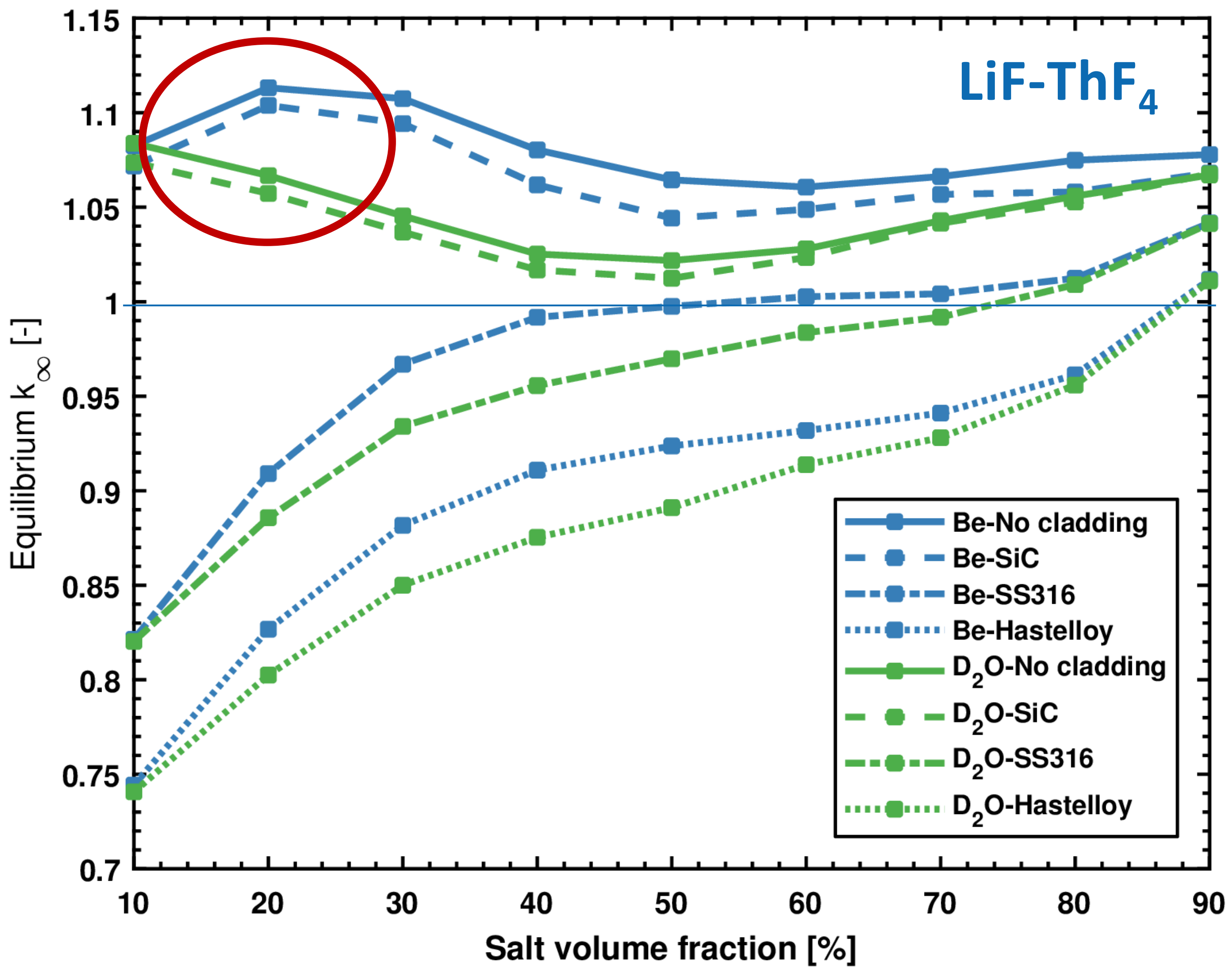
Neutronics impact of cladding (^{7}LiF salt example)

- **LiF salt** combined with **Be** and **D_2O** moderators was selected to analyze the impact of cladding:

  Hastelloy,
  SS316,
  and SiC.

- Only **SiC** seems to have acceptable low parasitic neutron capture.
- Purely from neutronics perspective **H**eavy **W**ater **B**oiling MSR would work

  HWB-MSR ☺



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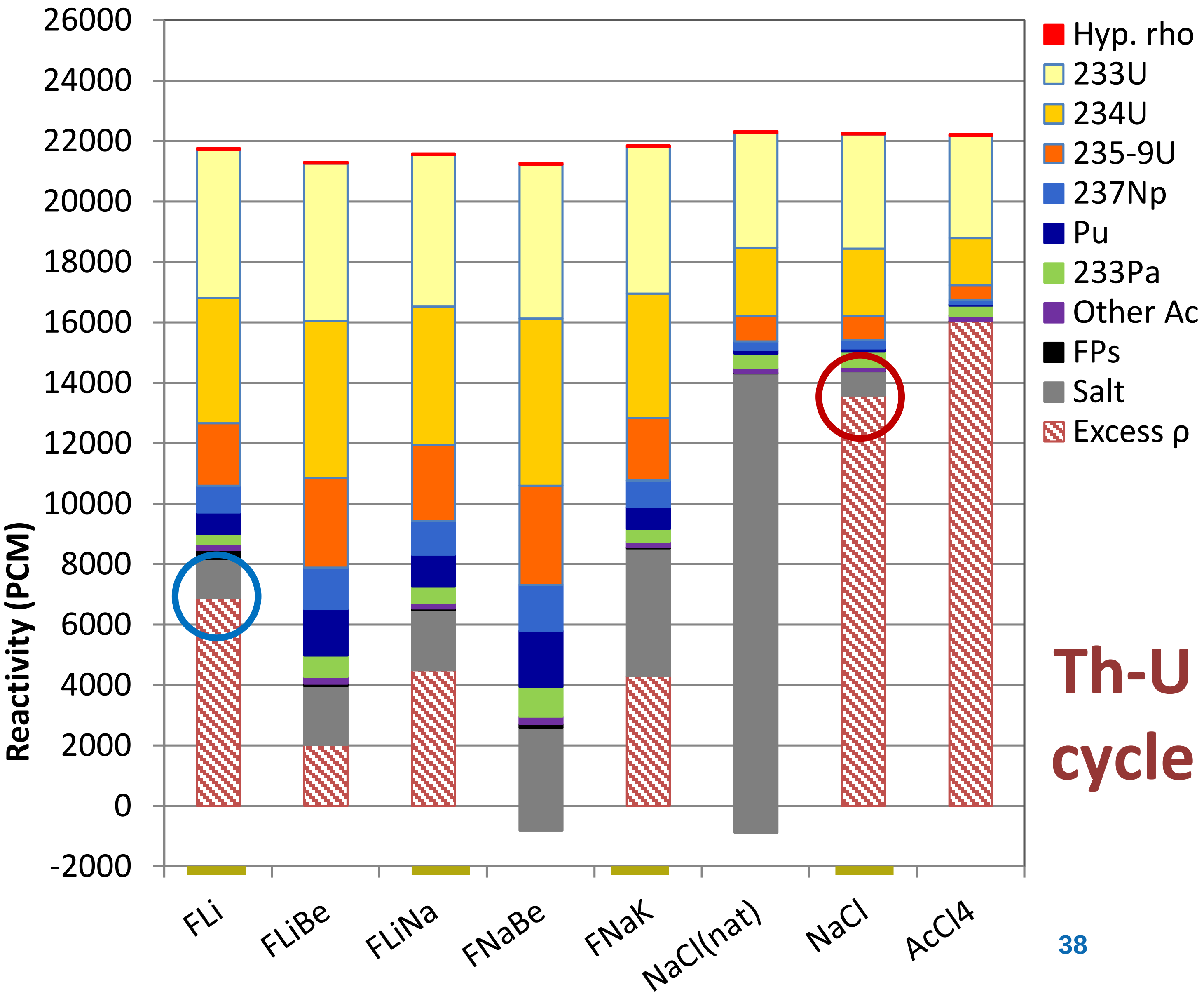
Hombourger, B.A., 2018. Ph.D. Thesis. EPFL Lausanne, Switzerland.

Breeding capability of homogeneous fast MSRs

II.3 family for fluorides
II.4 family for chlorides

Th-U cycle performance without moderator

- **8 salts** were evaluated:
  FLi, FLiBe, FLiNa, FNaBe, FNaK,
  NaCl (nat), $Na^{37}Cl$, $Ac^{37}Cl$.
  32% $AcCl_3$ *32% $AcCl_3$* *100% $AcCl_4$*
- **4** options in **Th-U** (reasonable melting point and reactivity): FLi, FLiNa, FNaK, $Na^{37}Cl$.
- $Na^{37}Cl$ provides the highest excess in Th-U of 13000 pcm.
- FLi is best fluoride salt with 6000 pcm.



Th-U cycle

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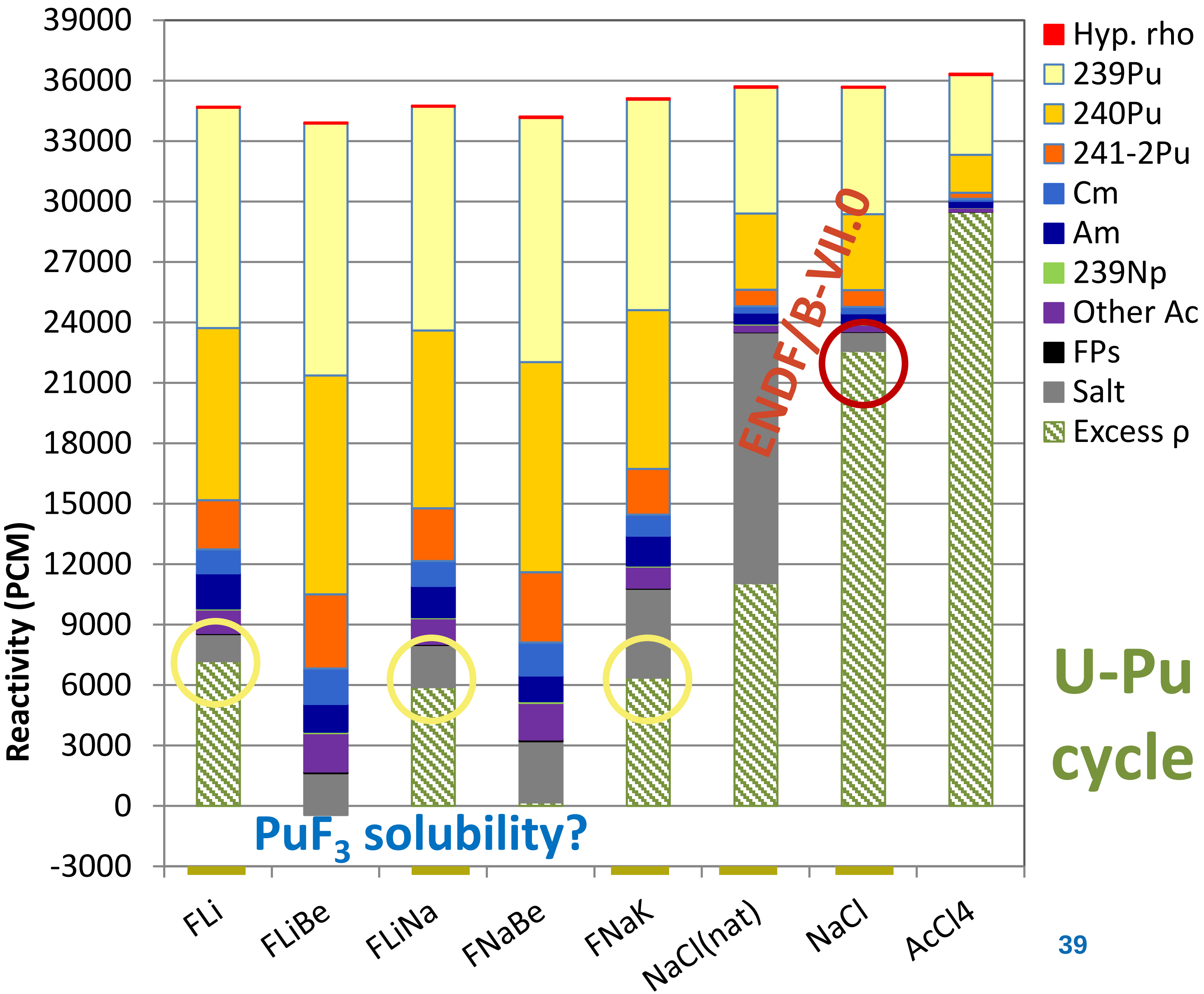
IAEA Technical Report Series, Status of Molten Salt Reactor Technology, document in preparation, International Atomic Energy Agency, 2021.

U-Pu cycle performance without moderator

- **8 salts** were evaluated:
  FLi, FLiBe, FLiNa, FNaBe, FNaK,
  NaCl (nat), $Na^{37}Cl$, $Ac^{37}Cl$.
  32% $AcCl_3$ 32% $AcCl_3$ 100% $AcCl_4$
- **5** options in **U-Pu** (reasonable melting point and reactivity):
  FLi, FLiNa, FNaK, NaCl (nat), $Na^{37}Cl$.
- **$Na^{37}Cl$** provides the highest overall excess of 22000 pcm.
- **FLi, FLiNa, FNaK** have similar performance of ~6000pcm, PuF_3 solubility is the major limiting issue.

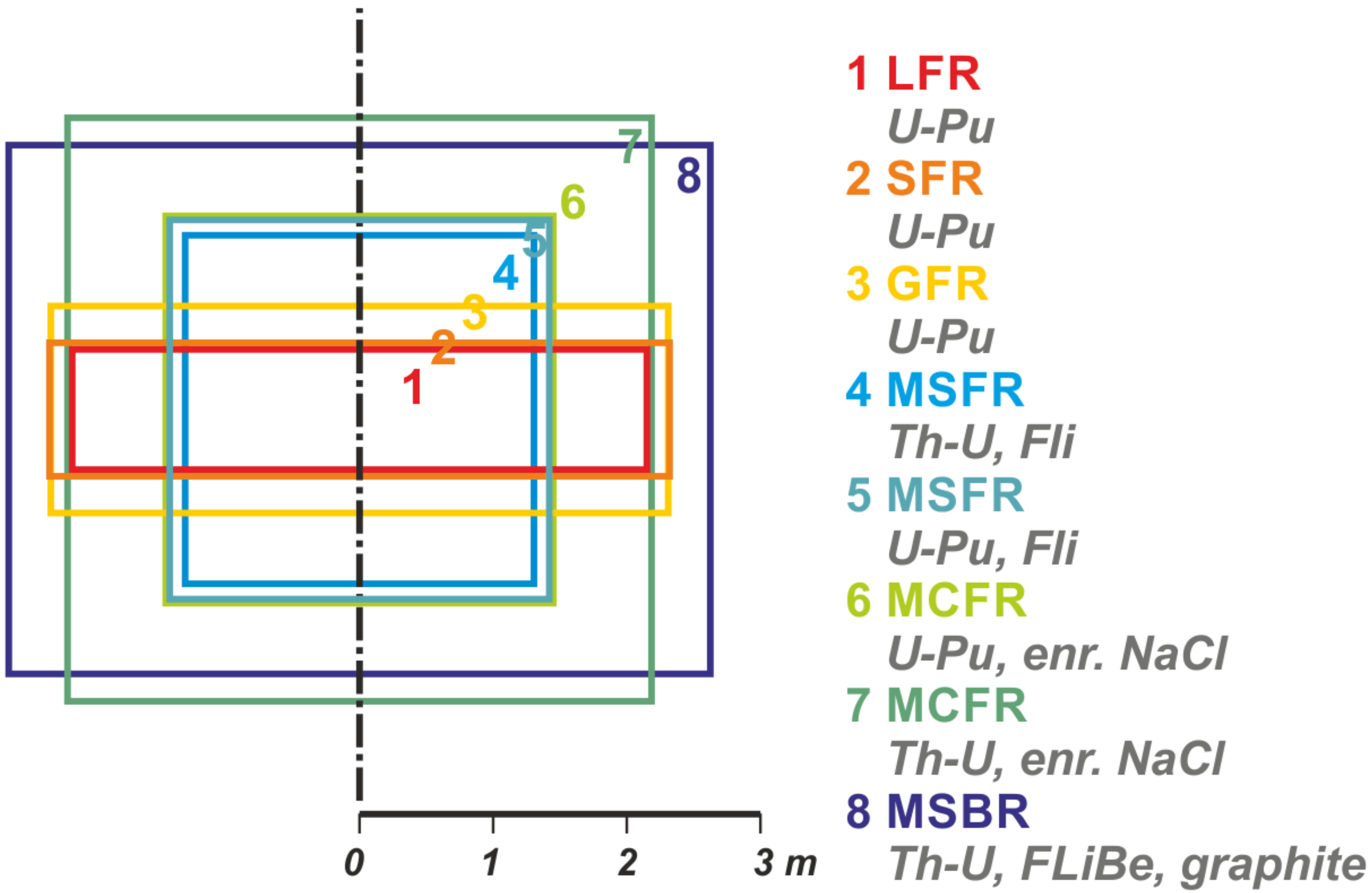


IAEA Technical Report Series, Status of Molten Salt Reactor Technology, document in preparation, International Atomic Energy Agency, 2021.

Self-sustaining breeder core size estimate

Self-sustaining breeder in closed cycle

- Using 1m **Hastelloy reflector** core size was estimated for **single-fluid** designs.
- It was compared with classical fast reactors.
- MSFR (**Fli**) in Th-U (4) is compact.
- MSFR (**Fli**) in U-Pu (5) is bigger.
- MCFR (**Na^{37}Cl**) in U-Pu (6) is comparable to MSFR in U-Pu (5).
- MCFR (**Na^{37}Cl**) in Th-U (7) is big.
- MSBR (ORNL design, 13% salt).



Hombourger, B.A., 2018. Ph.D. Thesis. EPFL Lausanne, Switzerland.

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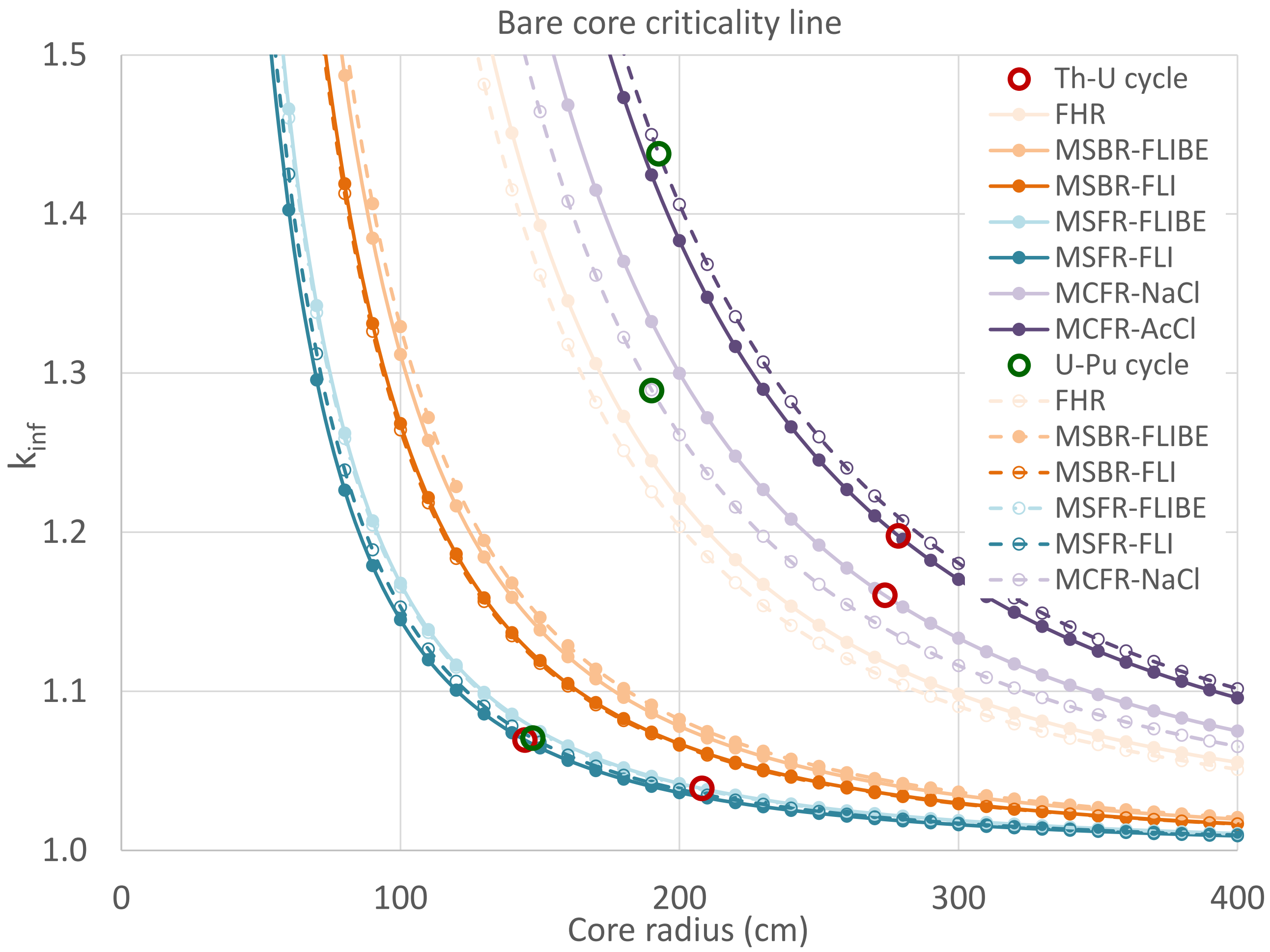

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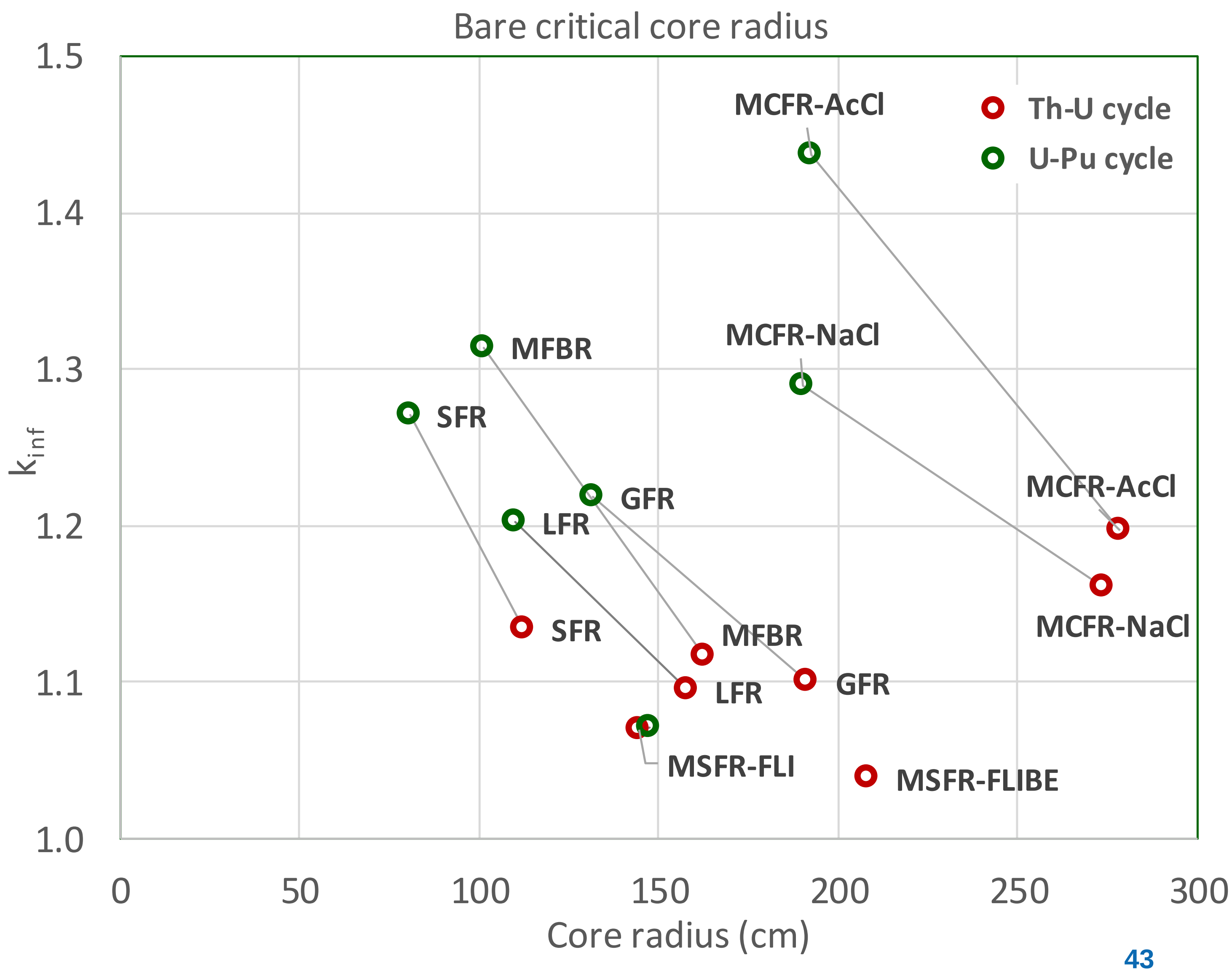
Core radius estimate: Th-U cycle X U-Pu cycle

- MSFR with Li^7F is the smallest MSR core and it has the same core size for both cycles. (very soft fast spectrum)
- By all other fast reactors U-Pu cycle provides smaller cores.
- SFR is the most compact bare iso-breeding core in both cycles.
- MCFR is the biggest bare iso-breeding core in both cycles.
- MSFR with BeF_2-Li^7F is subcritical for U-Pu cycle.



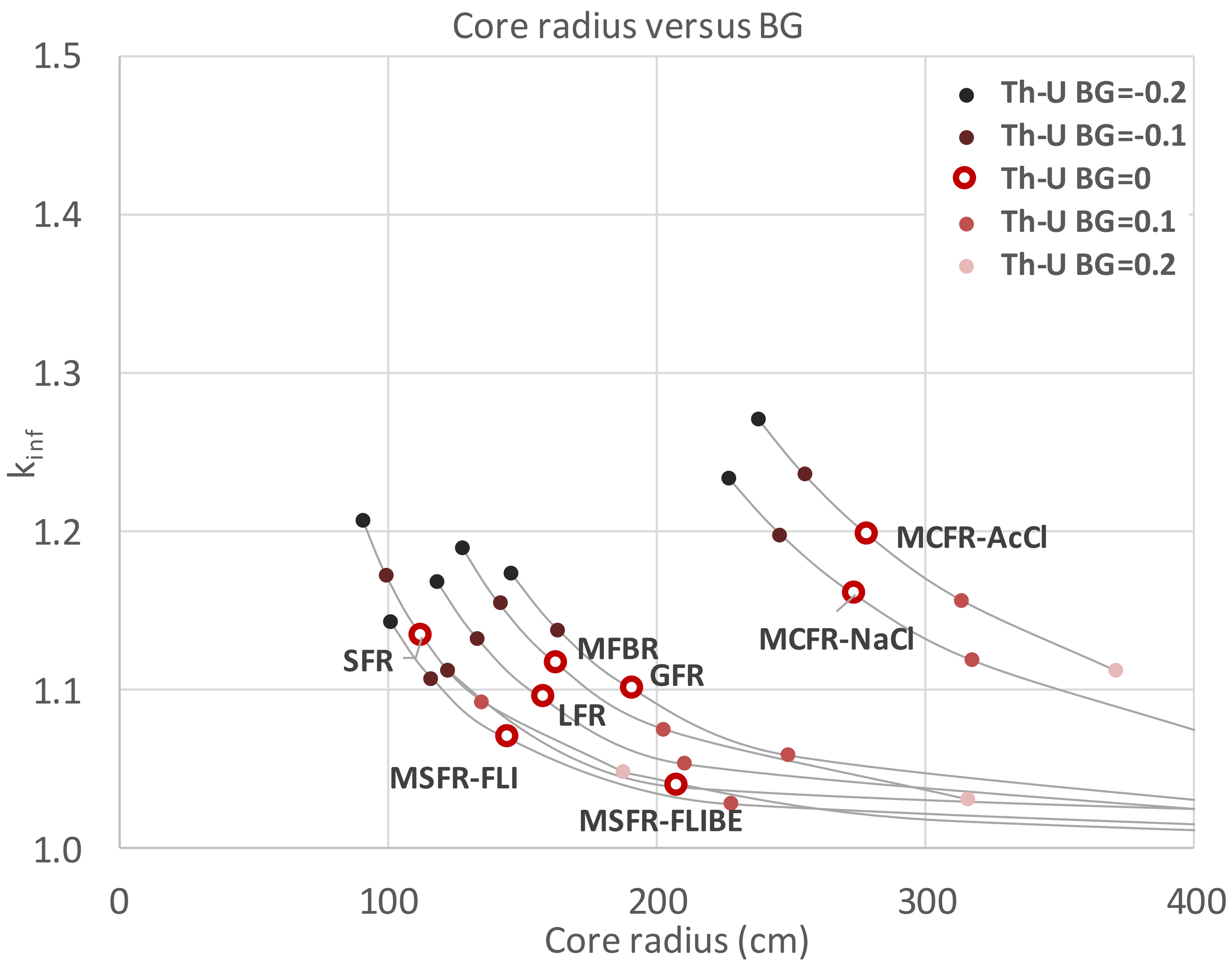
Core radius estimate in Th-U cycle

- Combining these two equations:

$$k_{eff} \cong k_{\inf} \frac{1}{1+M^2B^2}$$

$$BG_{per} \cong \bar{\nu}\, \frac{k_{\mathrm{eff}}-1}{k_{\mathrm{eff}}}$$

- Bare core size can be estimated for several BG values. **Th-U cycle =>**



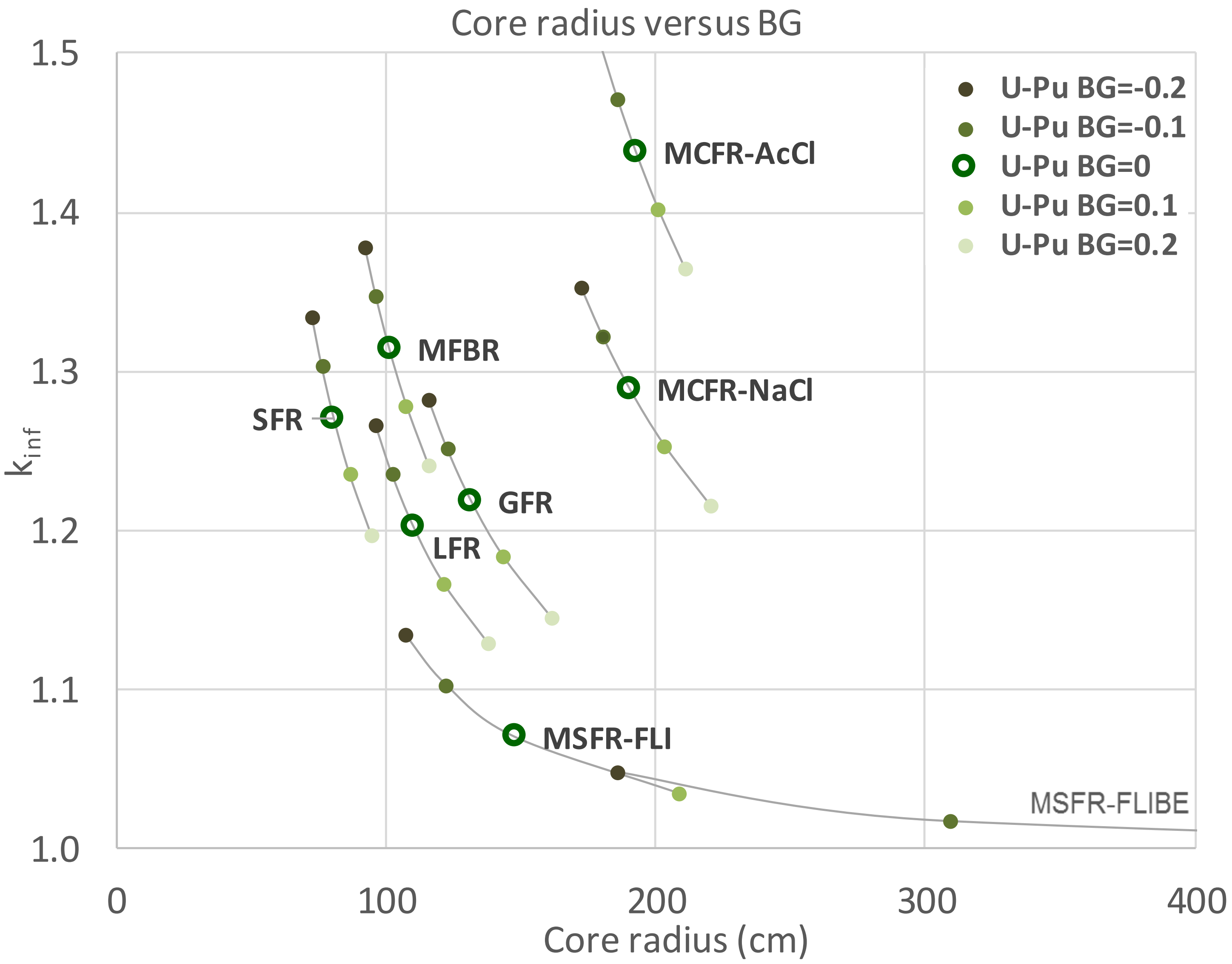
Core radius estimate in U-Pu cycle

- Combining these two equations:

$$k_{eff} \cong k_{\inf} \frac{1}{1+M^2B^2}$$

$$BG_{per} \cong \bar{\nu}\,\frac{k_{\mathrm{eff}}-1}{k_{\mathrm{eff}}}$$

- Bare core size can be estimated for several BG values. **U-Pu cycle =>**



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Self-sustaining breeding in open cycle (B&B)

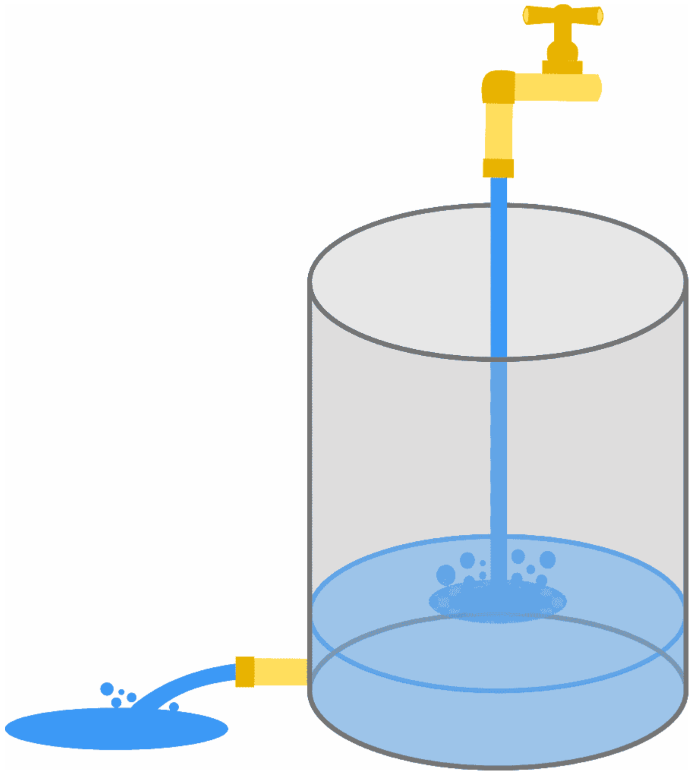
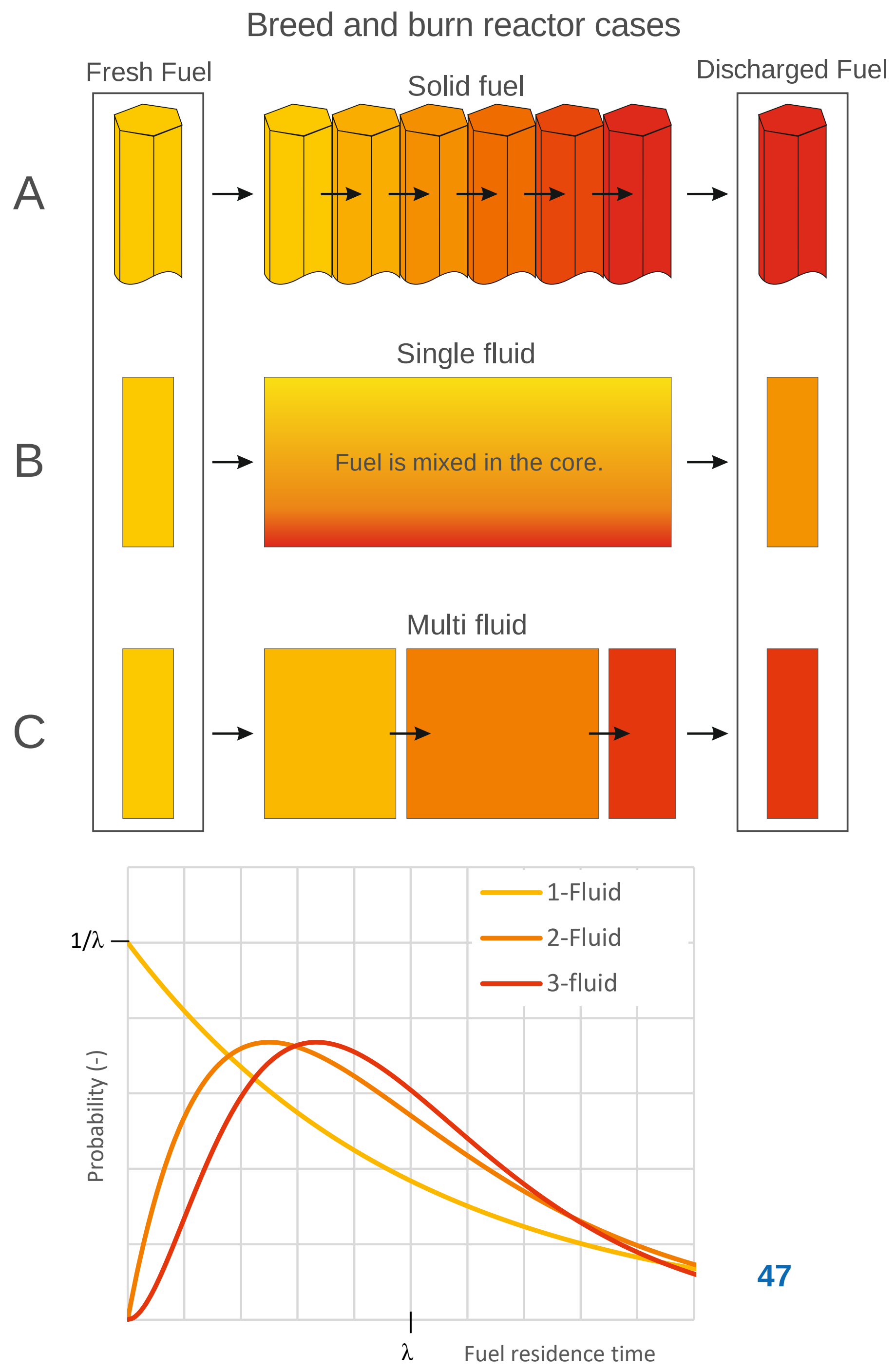


Illustration of tap-like reactor
https://www.subpng.com/

Breed & Burn cycle and burnup

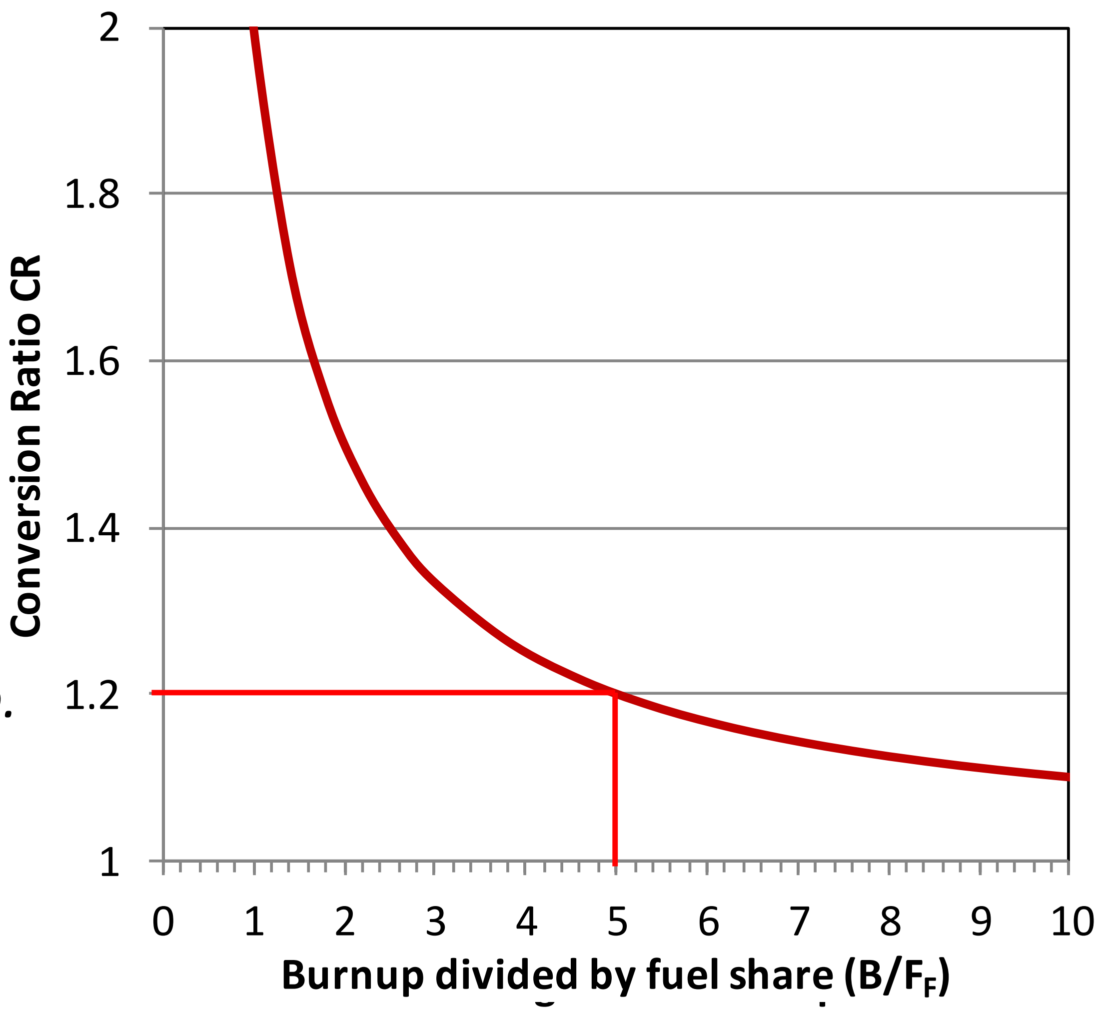
- Initially fertile fuel will be loaded, then the fissile fuel will be bred and firstly later it will be burned.
- The B&B cycle in liquid fuel reactor substantially differs from solid fuel.
- Discharged fuel:
  Most burned in solid fuel case
  Average burned in liquid fuel case.
- There is fuel residence time distribution=>
- To increase the burnup and reduce the core size (single-fluid layout can be bulky), multi-fluid layout can be used.



Trivial criteria for breed-and-burn cycle operation

- In B&B cycle conditions:
  1) fresh fuel is only fertile material
  2) spent fuel is not recycled.
- B&B trivial criterion (tautology): **I = II**
  I: Fissile Fuel $\mathbf{F_F}$ share in the discharged fuel.
  II: New fissile fuel bred in the discharged fuel.
- $$F_F = B(CR-1) \Rightarrow \frac{1}{CR-1} = \frac{B}{F_F}$$

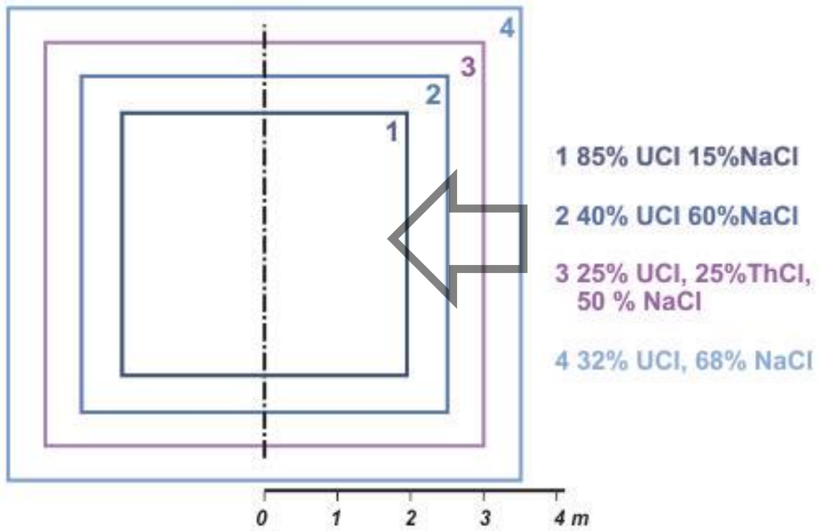
  where CR is conversion ratio and B is the fuel burnup.
- Reactor must be critical for CR, F_F, and B,
  e.g. for CR=1.2: F_F=10% ⇔ B=50% (1% ⇔ 5%)
- Fuel utilization in B&B cycle?
  It is equal to the burnup.

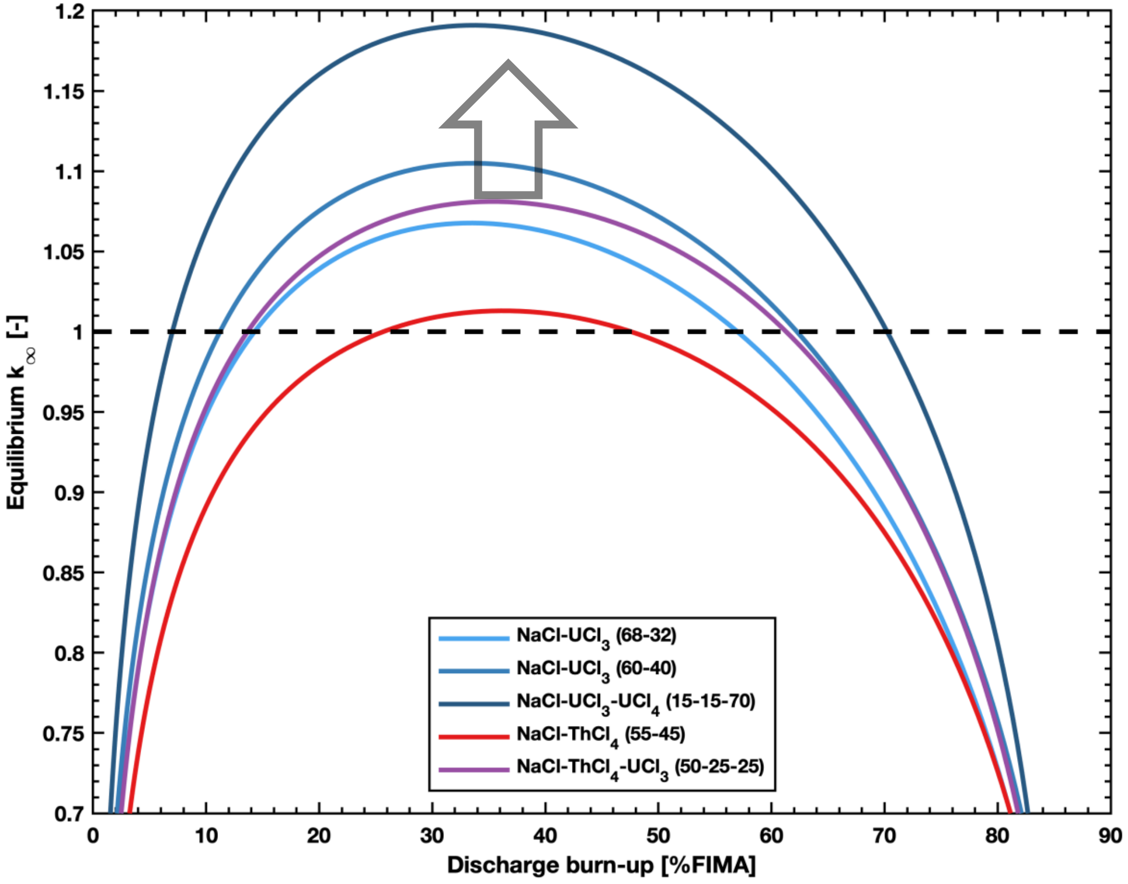


J. Krepel, B. Hombourger, E. Losa, Fuel cycle sustainability of Molten Salt Reactor concepts in comparison with other selected reactors, PHYTRA4, Marrakech, Morocco, September 17-19, 2018.

Self-sustaining breeder in open cycle (B&B)

- B&B is practically not possible in Th-U cycle.
- It is only possible in mixed U-Pu & Th-U cycle.
- B&B cores are bulky (chlorides = hard spectrum, but also high Migration area).
- The performance increases with growing actinides share in the core.

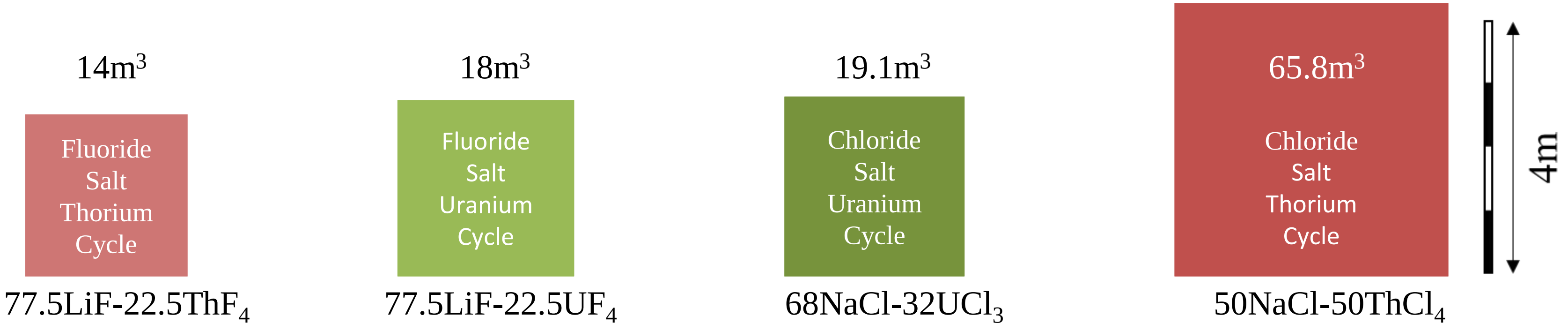




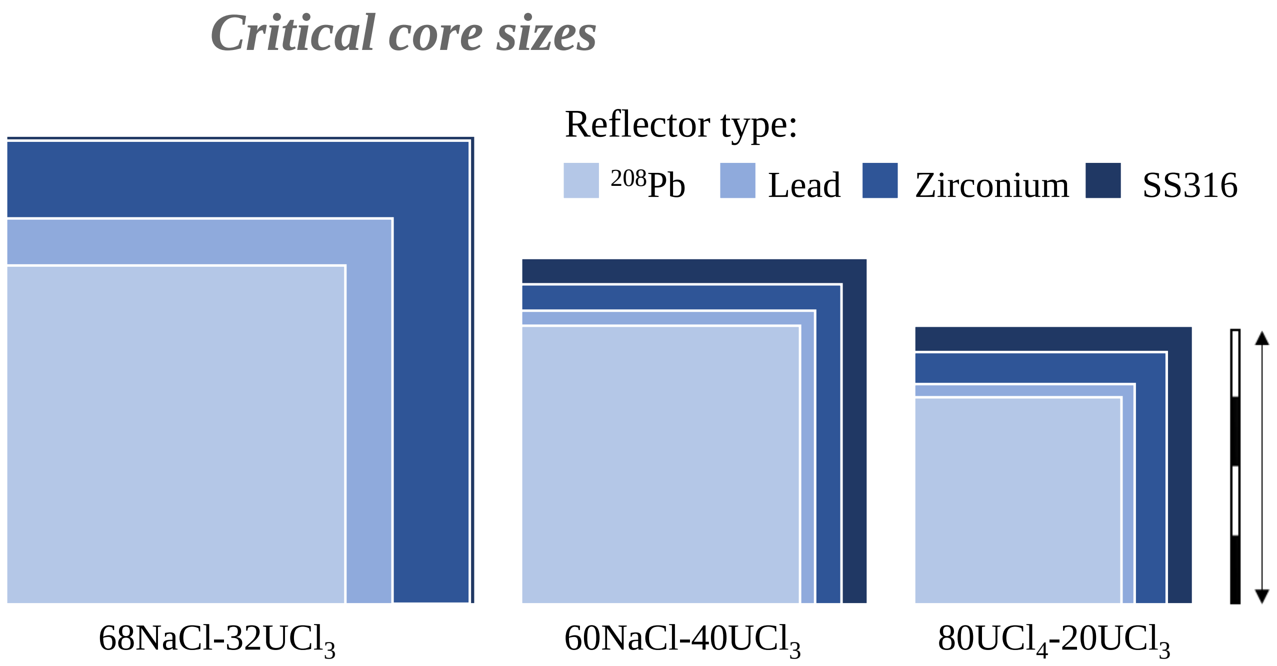
Hombourger, B. et al., 2019. Breed-and-Burn Fuel Cycle in Molten Salt Reactors. Submitted to special MSR edition of The European Physical Journal

Core size comparison for closed and open B&B cycle

- Closed cycle



- Breed and burn open cycle



Hombourger, B.A., 2018. Ph.D. Thesis. EPFL Lausanne, Switzerland.

Burnup definition

Burnup definition

- For solid fuel burnup is defined as:

$$B_{GWd/tHM}(t)=\frac{\int_0^t P(t)\,dt}{M_{Ac}(0)}$$

$$B_{FIMA\%}(t)=\frac{\int_0^t F(t)\,dt}{N_{Ac}(0)}$$

$$FPs_{share}=\frac{M_{FPs}(t)}{M_{Ac}(0)}=\frac{M_{FPs}(t)}{M_{Ac}(t)+M_{FPs}(t)}=B_{FIMA\%}(t)$$

- For liquid fuel two definitions are possible:
- Differential

$$B_{GWd/tHM}(t)=\frac{P(t)}{\dot{M}_{Ac,in}(t)}$$

$$B_{FIMA\%}(t)=\frac{F(t)}{\dot{N}_{Ac,in}(t)}\cong\frac{\dot{N}_{Ac,in}(t)-\dot{N}_{Ac,out}(t)}{\dot{N}_{Ac,in}(t)}\cong\frac{\dot{N}_{FPs,off-gas}(t)+\dot{N}_{FPs,out}(t)}{\dot{N}_{Ac,in}(t)}$$

- Integral

$$B_{GWd/tHM}(t)=\frac{\int_0^t P(t)\,dt}{M_{Ac,core}(0)+\int_0^t \dot{M}_{Ac,in}(t)\,dt}$$

$$B_{FIMA\%}(t)=\frac{\int_0^t F(t)\,dt}{N_{Ac,core}(0)+\int_0^t \dot{N}_{Ac,in}(t)\,dt}=\frac{\int_0^t F(t)\,dt}{N_{Ac,core}(t)+\int_0^t \dot{N}_{Ac,out}(t)\,dt+\int_0^t F(t)\,dt}$$

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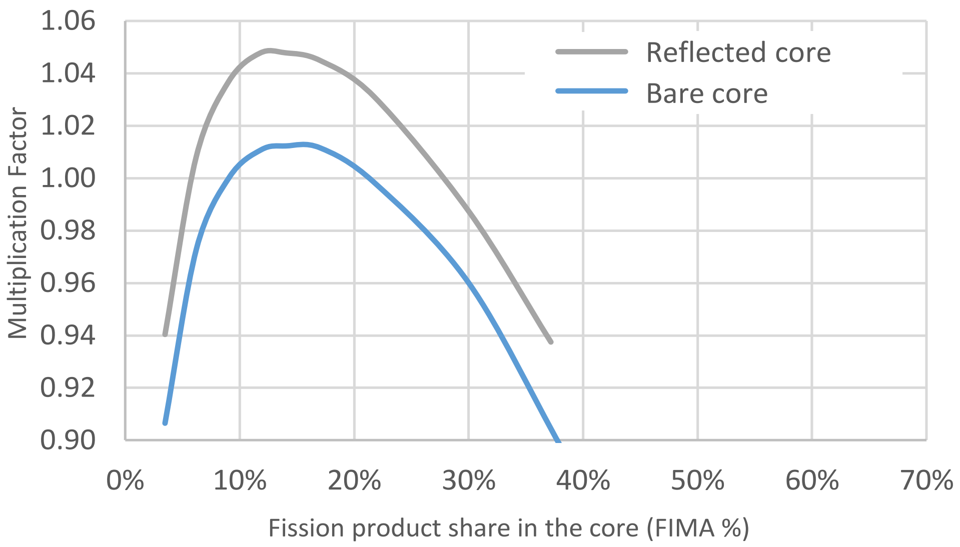
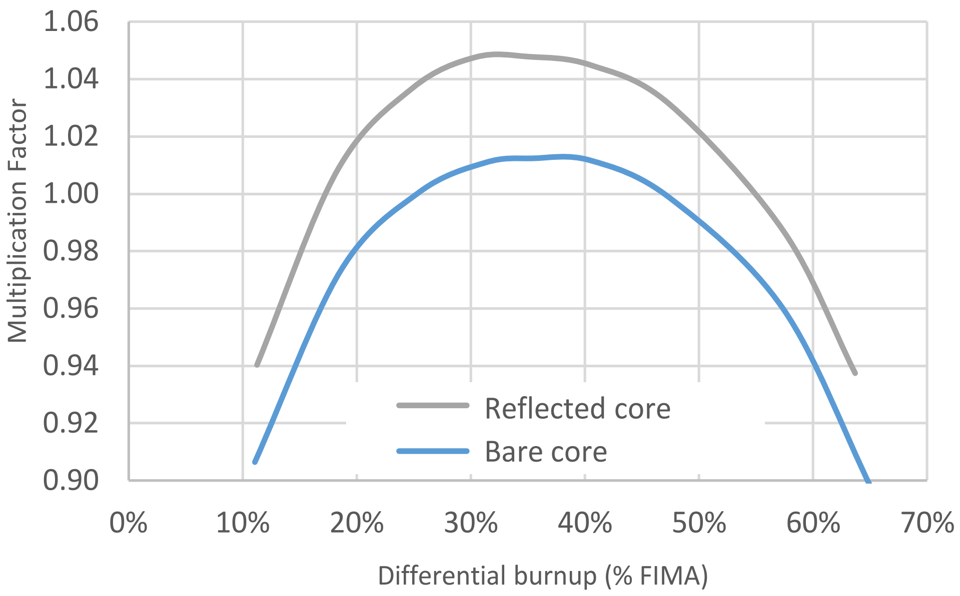
Burnup definition

- Due to the continuous FPs removal by off-gas system, the burnup and the fission products share in the core differs.

$$FPs_{share,core} = \frac{M_{FPs,core}(t)}{M_{Ac,core}(t) + M_{FPs,core}(t)} \neq B_{FIMA\%}(t)$$





Santora, J., 2022, Assessment of core minimization options for breed-and-burn molten chloride fast reactors, MSc thesis, EPFL Lausanne.

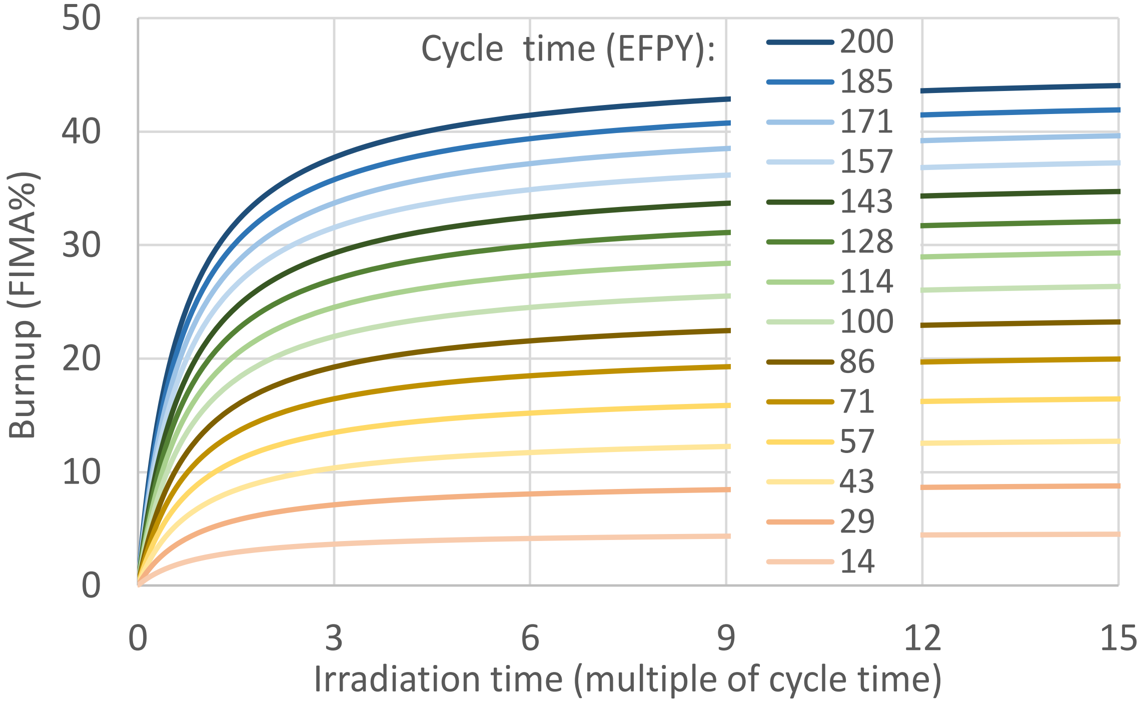
Burnup definition

- The differential and integral definition provide different values.
- The integral definition includes the initial core loading.
- For stabilized and long enough operation, they can be equal.

$$B_{GWd/tHM}(t) = \frac{P(t)}{\dot{M}_{Ac,in}(t)}$$

$$\Updownarrow$$

$$B_{GWd/tHM}(t) = \frac{\int_0^t P(t)\,dt}{M_{Ac,core}(0) + \int_0^t \dot{M}_{Ac,in}(t)\,dt}$$

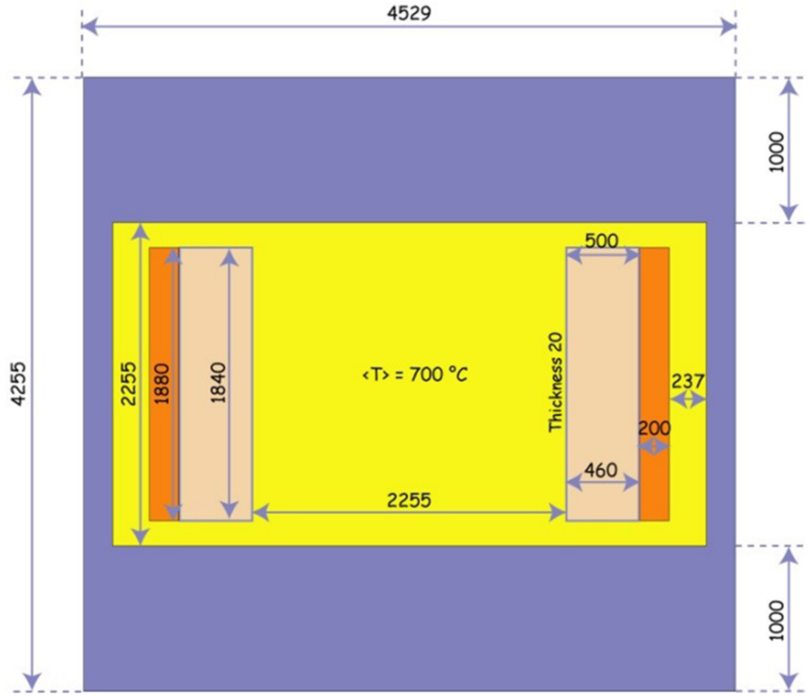


Krepel, J., et al., 2022, Characterization of the Molten Chloride Fast Reactor fuel cycle options, proceedings of FR22, IAEA.

Radionuclides distribution and release during accidental conditions

Fuel reprocessing

- Many MSR concepts rely on gaseous FPOs removal and fuel salt reprocessing.
- As an example the EVOL and MARS projects benchmark is taken here.
- The active core is divided into blanket and fuel salt.
- Gaseous and volatile FPs
  Z = 1, 2, 7, 8, 10, 18, 36, 41, 42, 43, 44, 45, 46, 47, 51, 52, 54 and 86
  are removed with 30s cycle time.
- **For later use**: Zr (Z=40) is not included in volatile FPs.
- Fuel salt is reprocessed with cycle time of 450 days:
  Z = 30, 31, 32, 33, 34, 35, 37, 38, 39, 40, 48, 49, 50, 53, 55, 56, 57, 58, 59, 60, 61, 62, 63, 64, 65, 66, 67, 68, 69, 70



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Brovchenko, M., et al,. 2019, Ph.D. Neutronic benchmark of the molten salt fast reactor in the frame of the EVOL and MARS collaborative projects, EPJ Nuclear Sci. Technol.

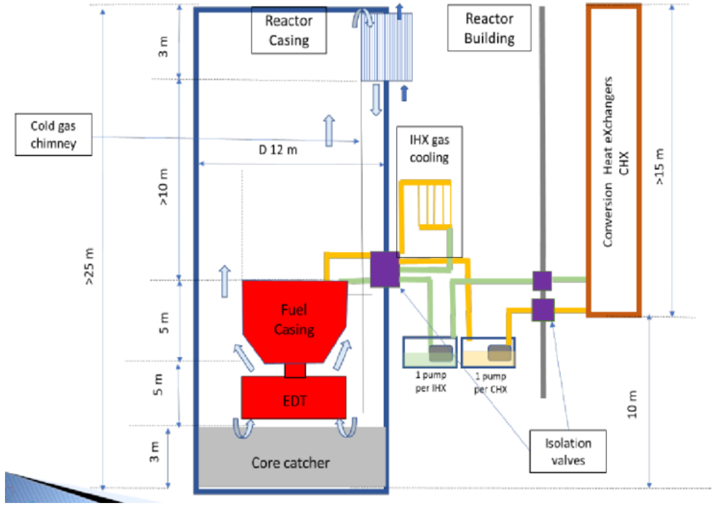
Radiotoxicity distribution in core, blanket, reprocessing unit and off-gas system.

Ingestion radiotoxicity after 200 EFPD of operation per 1 m^3 of core volume divided into FPs chains and zones.

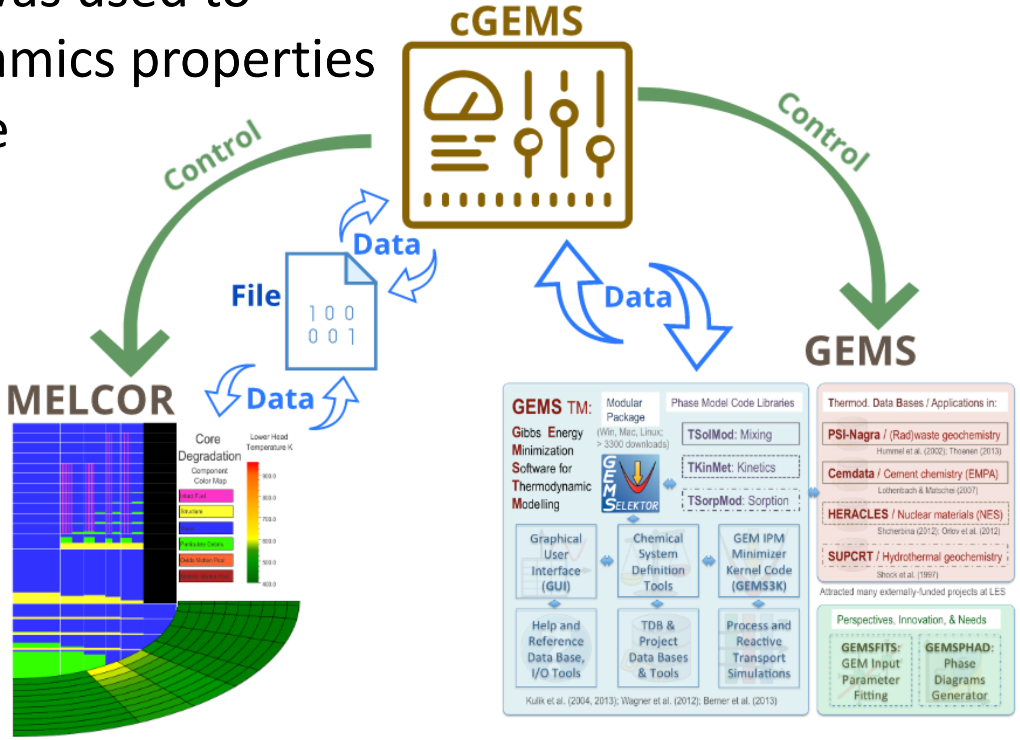
Rank	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
Atomic number	133	85	88	135	129	130	87	131	127	138	233	105	143	84	125
Nuclides	133In 133Sn 133Sb 133Te-m 133Te 133I 133Xe-m 133Xe	85Ga 85Ge 85As 85Se-m 85Se 85Br 85Kr-m 85Kr	88Ge 88As 88Se 88Br 88Kr 88Rb 88Sr	135Sn 135Sb 135Te 135I 135Xe-m 135Xe 135Cs	129In-m 129In 129Sn-m 129Sn 129Sb 129Te-m 129Te 129I	130Pd 130Ag 130Cd 130In 130Sn 130Sb-m 130Sb 130Te	87Ge 87As 87Se 87Br 87Kr 87Rb 87Sr-m	131Cd 131In 131Sn 131Sb 131Te-m 131Te 131I 131Xe-m	127Cd 127In-m 127In 127Sn-m 127Sn 127Sb 127Te-m 127Te	138Sn 138Sb 138Te 138I 138Xe 138Cs-m 138Cs	233Th 233Pa	105Zr 105Nb 105Mo 105Tc 105Ru 105Rh-m 105Rh	143Xe 143Cs 143Ba 143La 143Ce 143Pr 143Nd	84Zn 84Ga 84Ge 84As 84Se 84Br-m 84Br	125Ag 125Cd 125In-m 125In 125Sn-m 125Sn 125Sb 125Te-m
Half-lives	0.18s 1.44s 2.5m 55.4m 12.4m 20.8h 2.19d 5.243d	0.087s 0.250s 2.03s 19s 39s 2.87m 4.48h 10.73y	0.129s 0.135s 1.50s 16.4s 2.84h 17.7m stable	0.418s 1.71s 19.0s 6.57h 15.3m 9.10h 2.3e6y	1.23s 0.63s 6.9m 2.4m 4.40h 33.6d 1.16h 1.6e7y	- - 0.20s 0.29s 3.7m 6.5m 38.4m stable	0.134s 0.8s 5.6s 55.9s 1.27h 10.67l 2.81h	0.106s 0.28s 39s 23.0m 1.35d 25.0m 8.040d 11.9d	0.4s 3.73s 1.14s 4.15m 2.12h 3.84d 109d 9.4h	- 0.173s 1.4s 6.5s 14.1m 2.9m 32.2m	22m 27d	0.493s 3.0s 36s 7.6m 4.44h 40s 35.4h	0.30s 1.78s 14.3s 14.1m 1.38d 13.57d stable	- 0.098s 1.2s 5.5s 3.3m 6.0m 31.8m	0.334s 0.68s 12.2s 2.36s 9.5m 9.63d 2.758y 58d
Total ingestion radiotoxicity (Sv/m^3)	**2.1E+11**	**2.5E+11**	**2.1E+11**	**1.4E+11**	**1.4E+11**	**1.0E+11**	**4.6E+10**	**4.1E+10**	**2.7E+10**	**2.3E+10**	**1.3E+10**	**1.3E+10**	**1.1E+10**	**9.9E+09**	**8.7E+09**
Off-gas system (%)	**99.9**	**98.9**	**99.6**	**99.6**	**91.5**	**89.1**	**99.5**	**80.7**	**99.7**	**97.6**	0.0	**98.1**	0.0	**88.6**	**100.0**
Fuel in core (%)	0.1	**1.1**	0.4	0.4	**8.5**	**10.9**	0.5	**19.3**	0.3	**2.4**	**91.0**	**1.9**	**99.6**	**11.4**	0.0
Reproc. unit (%)	0.0	0.0	0.0	0.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.3	0.0	0.0
Fuel in blanket (%)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	**8.6**	0.0	0.1	0.0	0.0

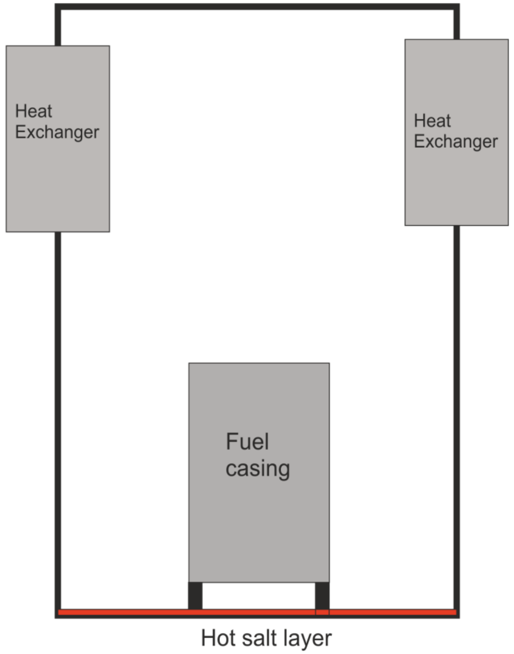
Simulation of severe accident in MSFR with salt spill

- Assuming simple scenario of fuel salt spill to the bottom of the containment the radiotoxicity released as vapour and aerosols can be calculated.
- Linear heat up of the salt to 1500K in 2 hours was assumed.
- PSI in-house code GEMS was used to calculate the thermo-dynamics properties and loosely coupled to the MELCORE core (cGEMS).
- GEMS relies on the HERACLES database.



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





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Kalilainen, J., et al., 2020, Evaporation of materials from the molten salt reactor fuel under elevated temperatures, https://doi.org/10.1016/j.jnucmat.2020.152134

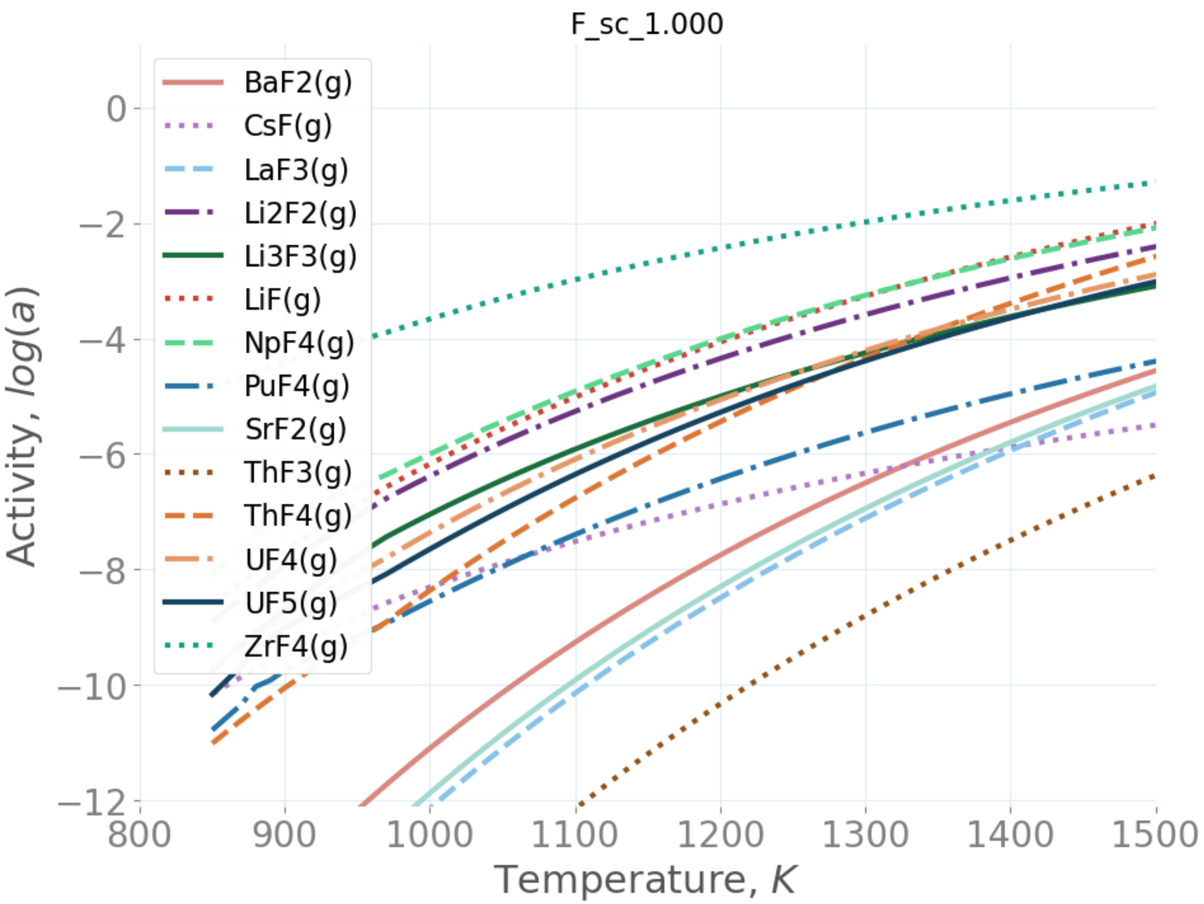
Heracles database extension

- The respective database for GEMS code was extended for the purpose of the simulation:

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

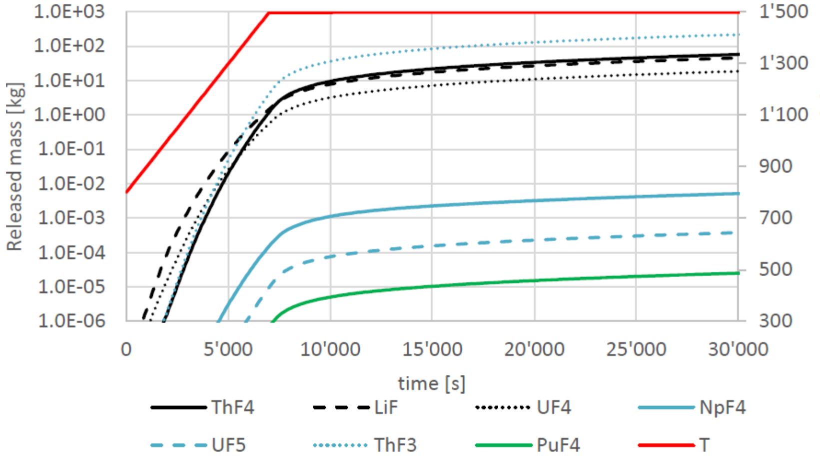


Compounds activity (proportional to vapor pressure) as a function of temperature

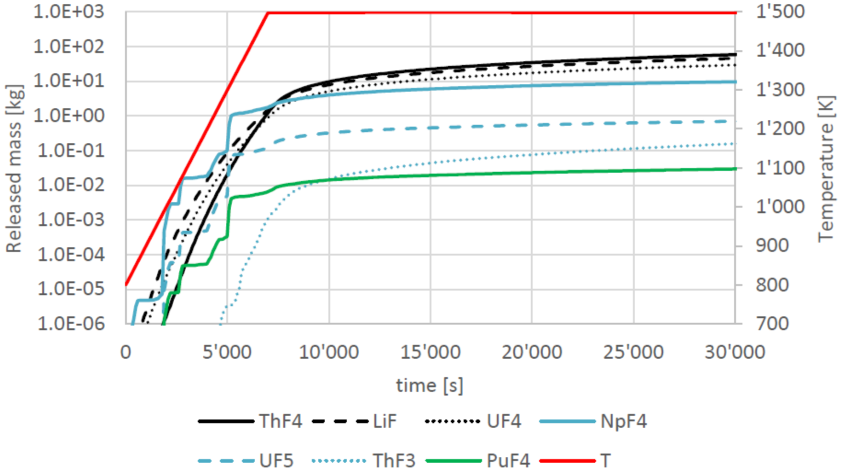
Dietz, J., et al., 2022, MSR fuel cycle and thermo-dynamics simulations, proceedings of FR22, IAEA.

Total released mass during the accident (salt heat up from 800°C to 1500°C)

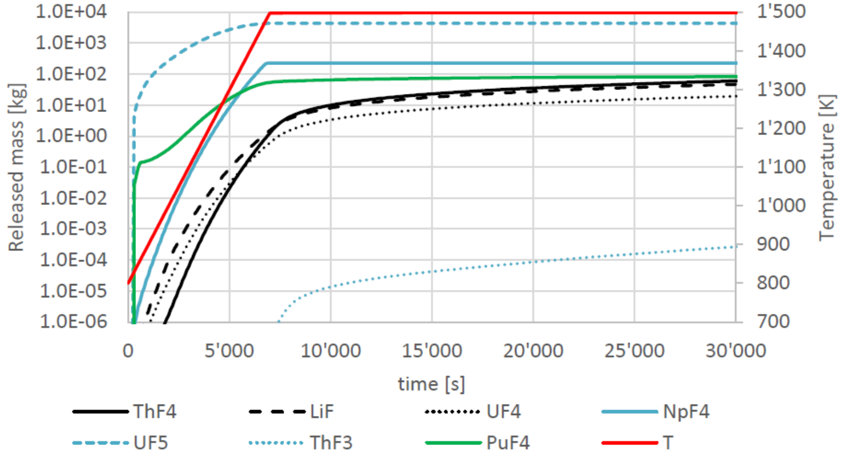
Fluorine: -1% mol.



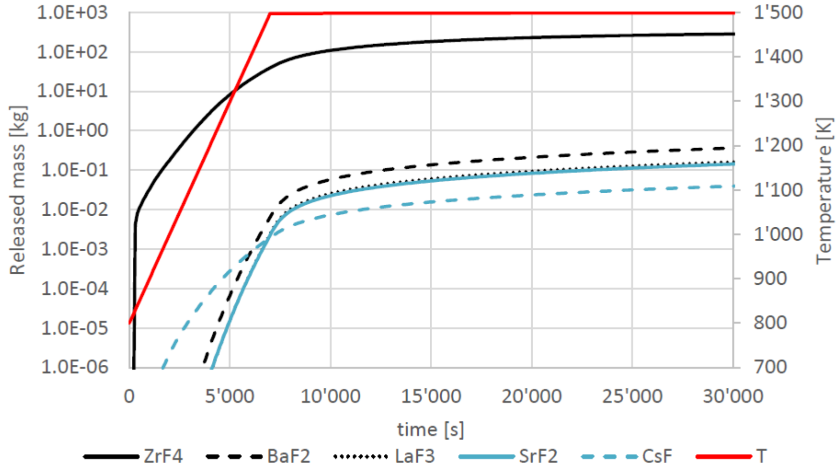
Stoichiometric

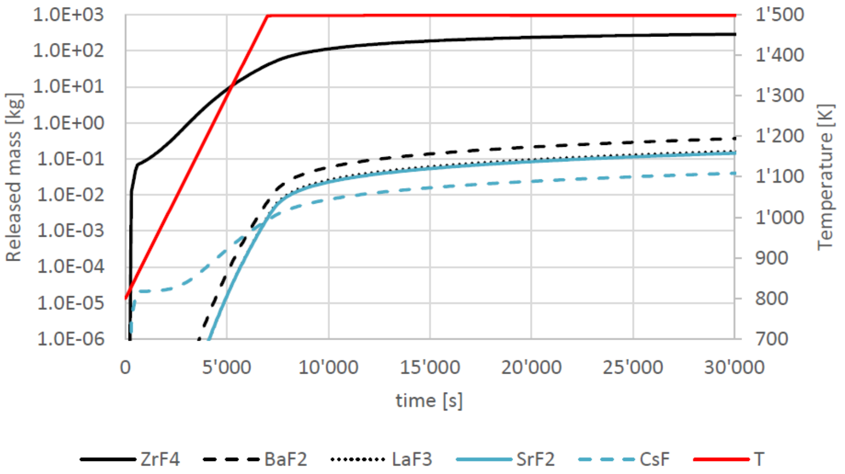


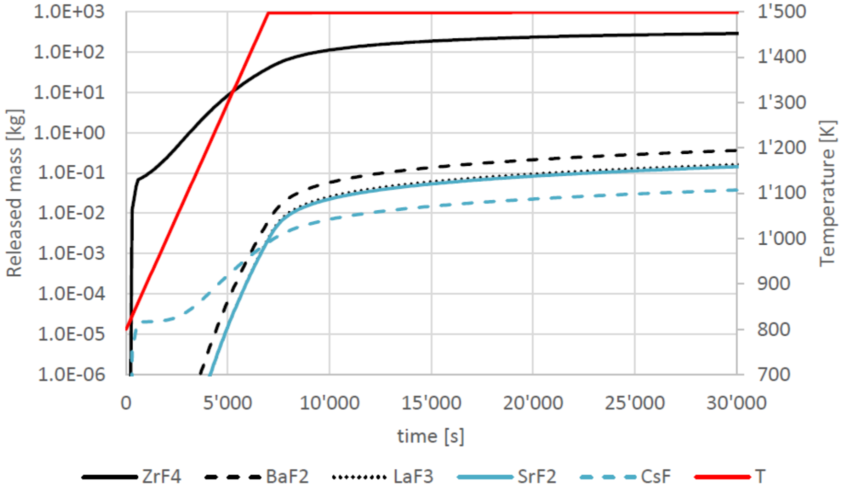
+1% mol.



Actinides and salt species



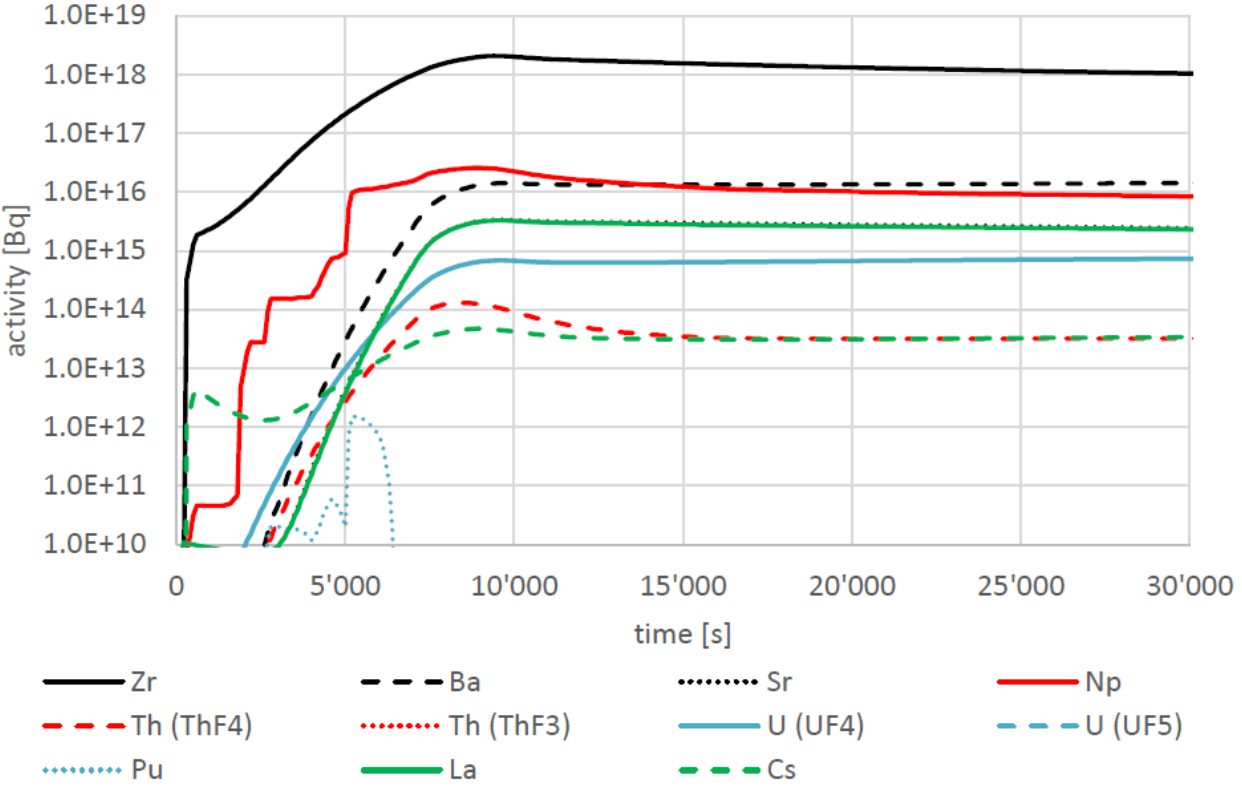


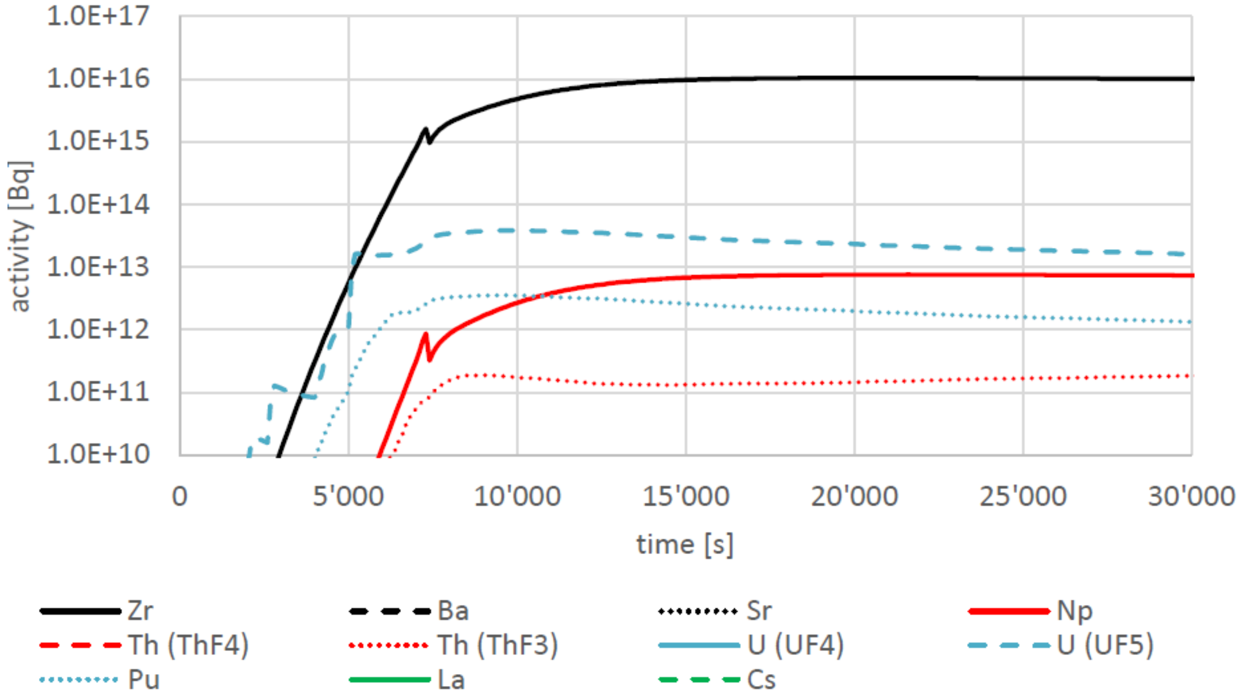


Fission products species

Kalilainen, J., et al., 2020, Evaporation of materials from the molten salt reactor fuel under elevated temperatures, https://doi.org/10.1016/j.jnucmat.2020.152134

Characterization of released activity in form of aerosols and vapors



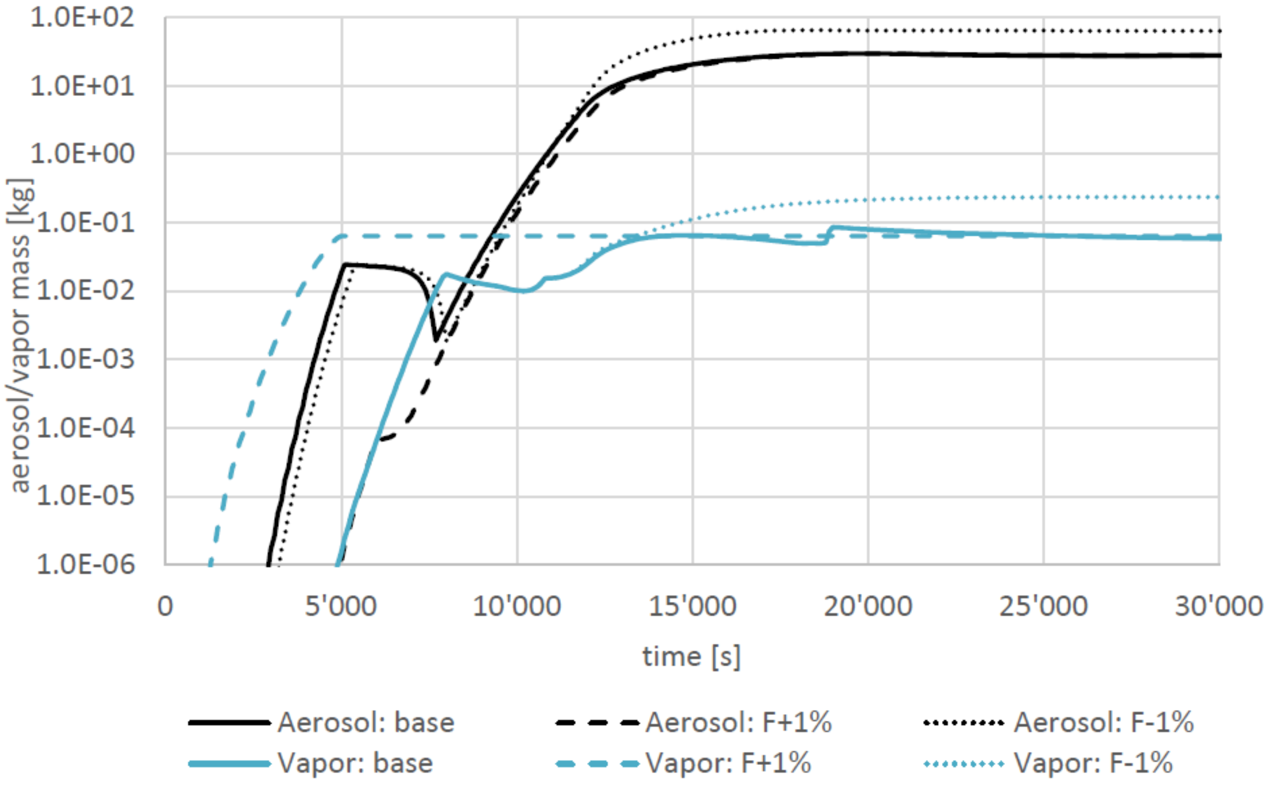


Total released activity in form of aerosols (left) and vapors (right) during the accident (salt heat up from 800°C to 1500°C)

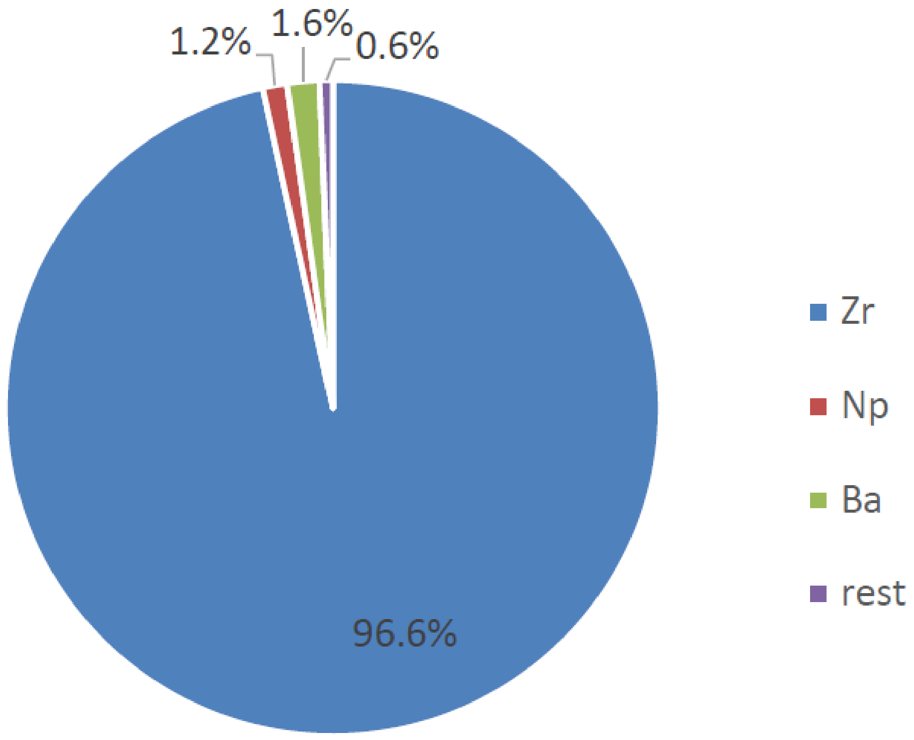
Kalilainen, J., et al., 2020, Evaporation of materials from the molten salt reactor fuel under elevated temperatures, https://doi.org/10.1016/j.jnucmat.2020.152134

Major radiotoxicity component

- Based on the applied benchmark reprocessing scheme, ZrF_4 in form of aerosols seems to be the major activity carrier during the postulated accident.

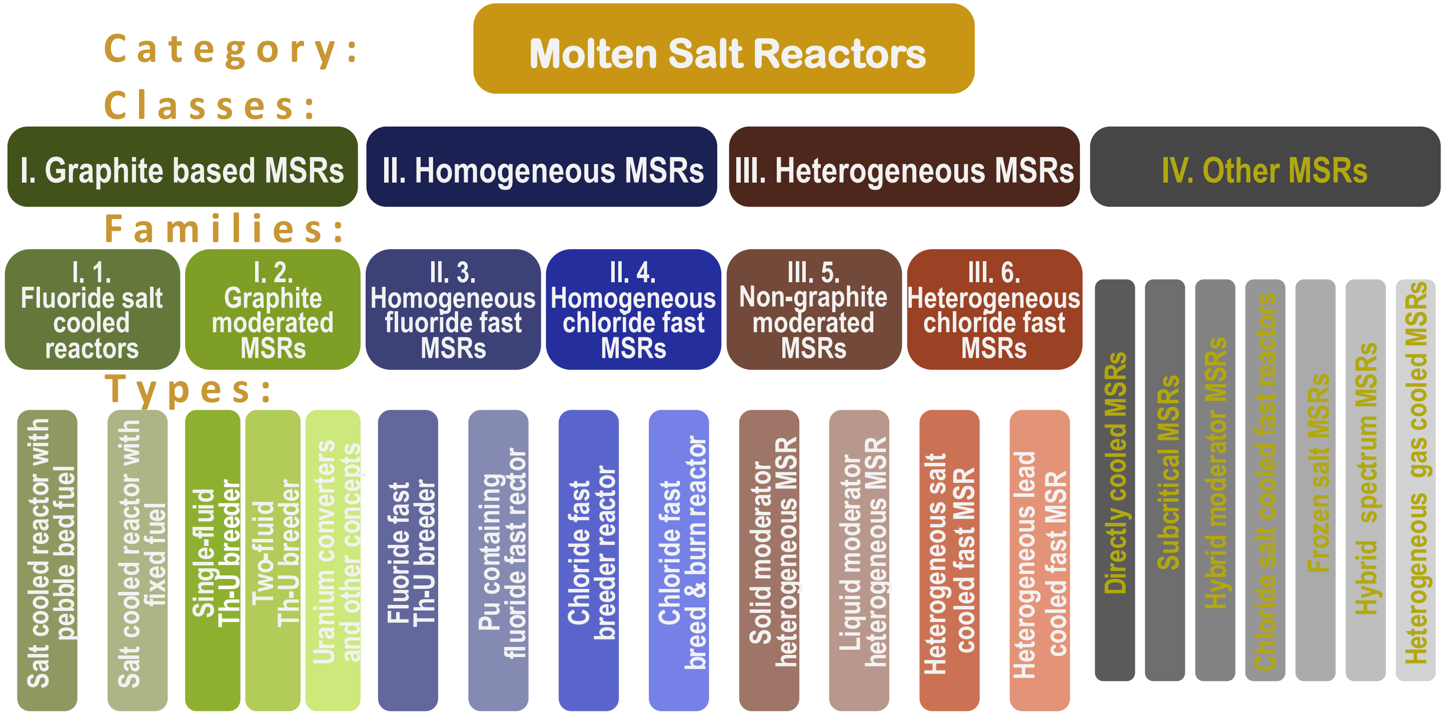


Total released activity in form of aerosols and vapors during the accident (salt heat up from 800°C to 1500°C)



Activity break-down at the end of simulation (t=30’000s) of the accident (salt heat up from 800°C to 1500°C)

Thank you for your attention



Adopted from: IAEA Technical Report Series, Status of Molten Salt Reactor Technology, document in preparation, International Atomic Energy Agency, 2021.

Upcoming Webinars

Date	Title	Presenter
22 February 2023	Safe Final Disposal of Spent Nuclear Fuel in Finland	Mr. Mika Pohjonen and Ms. Mari Lahti, Posiva, Finland
30 March 2023	Advanced Reactor Safeguards and Materials Accountancy Challenges	Dr. Ben Cipiti, Sandia National Laboratories, USA
05 April 2023	Overview of Nuclear Graphite R&D in Support of Advanced Reactors	Dr. Will Windes, Idaho National Laboratory, USA