PSI Center for Scientific Computing, Theory and Data

MSR R&D Activities in Switzerland

GIF MSR Workshop
PSI Auditorium Switzerland

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10 December 2025

MSR research in 70s and 80s

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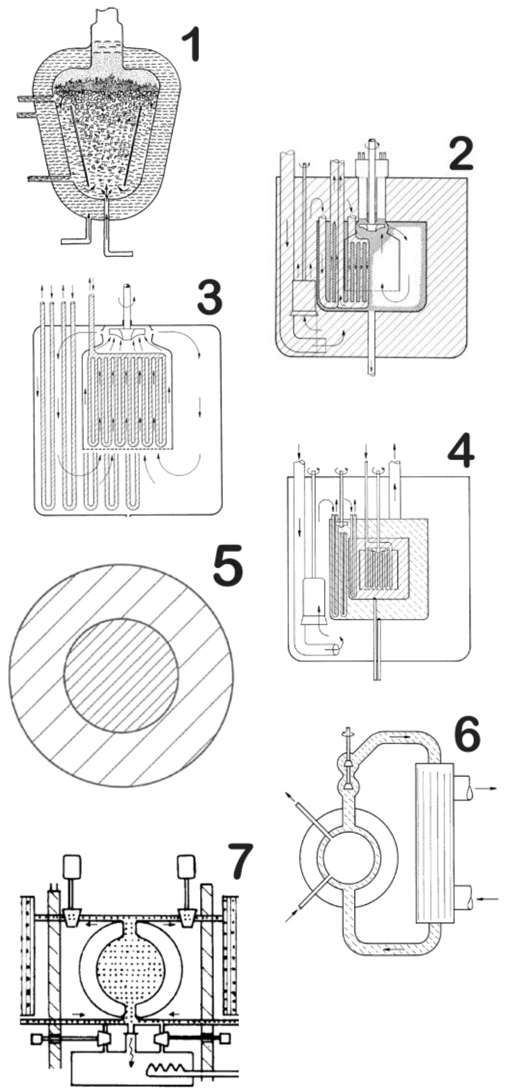
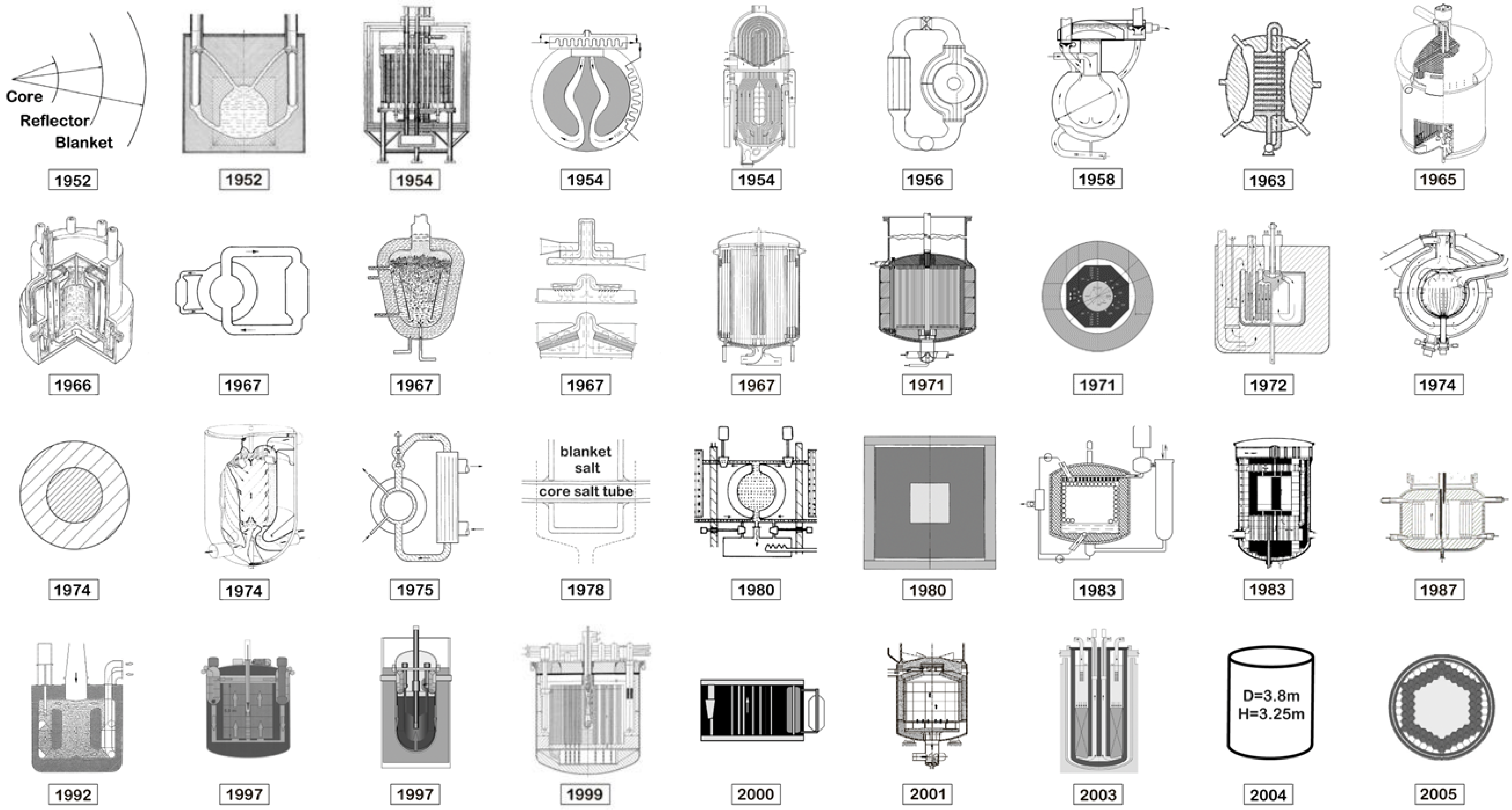
- In 70s and 80s the MSR research at EIR was led by **Prof. Taube**.
- Focusing on **chloride salts, breeding and waste minimizing.**

Nr.	Reference	Breeder / cycle	Fuel type	Blanket type	Primary coolant	Core layout / Moderator	Core shape
1	Taube et. al., 1967	Yes / U-Pu cycle	chloride salt	chloride salt	boiling $AlCl_3$	homogeneous / none	semi-spherical
2	Taube and Ligou, 1972, 1974; Taube , 1974A	Yes / U-Pu cycle	chloride salt with Pu	chloride salt with U	blanket salt	heterogeneous / none	cylindrical
3	Taube , 1974A	No / waste burner	chloride salt with Pu	salt with FPs and Be	salt with FPs and Be	heterogeneous / none	cylindrical
4	Taube , 1974A	Yes / waste burner	chloride salt with Pu	chloride salt with U	salt with FPs and Be	heterogeneous / none	cylindrical
5	Taube, 1974B	Yes / mixed cycle	chloride salt with U-Pu	chloride salt with Th-U	Fuel salt	homogeneous / none	spherical
6	Taube et al., 1975A, 1975B	No / waste burner	chloride salt in outer speher	central waste burning zone	Fuel salt	intermediate Be moderator loop	spherical
7	Taube and Heer, 1980	Yes / U-Pu cycle	chloride salt	none	Fuel salt	reflected by chloride salt	spherical



Adopted from: KREPEL, J., KRAMER, K., J., Molten Chloride Fast Reactors (MCFRs), Encyclopedia of Nuclear Energy (Greenspan, E., Ed.), Elsevier, 2021

MSR Taxonomy



Prof. Taube proposed in 1978 MSR taxonomy

In 1978 EIR (PSI) final report was published with MSR classification based predominantly on cooling method. It was biased towards fast MSR and strongly included directly cooled MSR.

1.1 Methods of classification

There are many ways of classifying a reactor type. One such possibility is shown here.

a) Method of cooling

b) Flux intensity related also to specific power density

c) Number of zones in the reactor

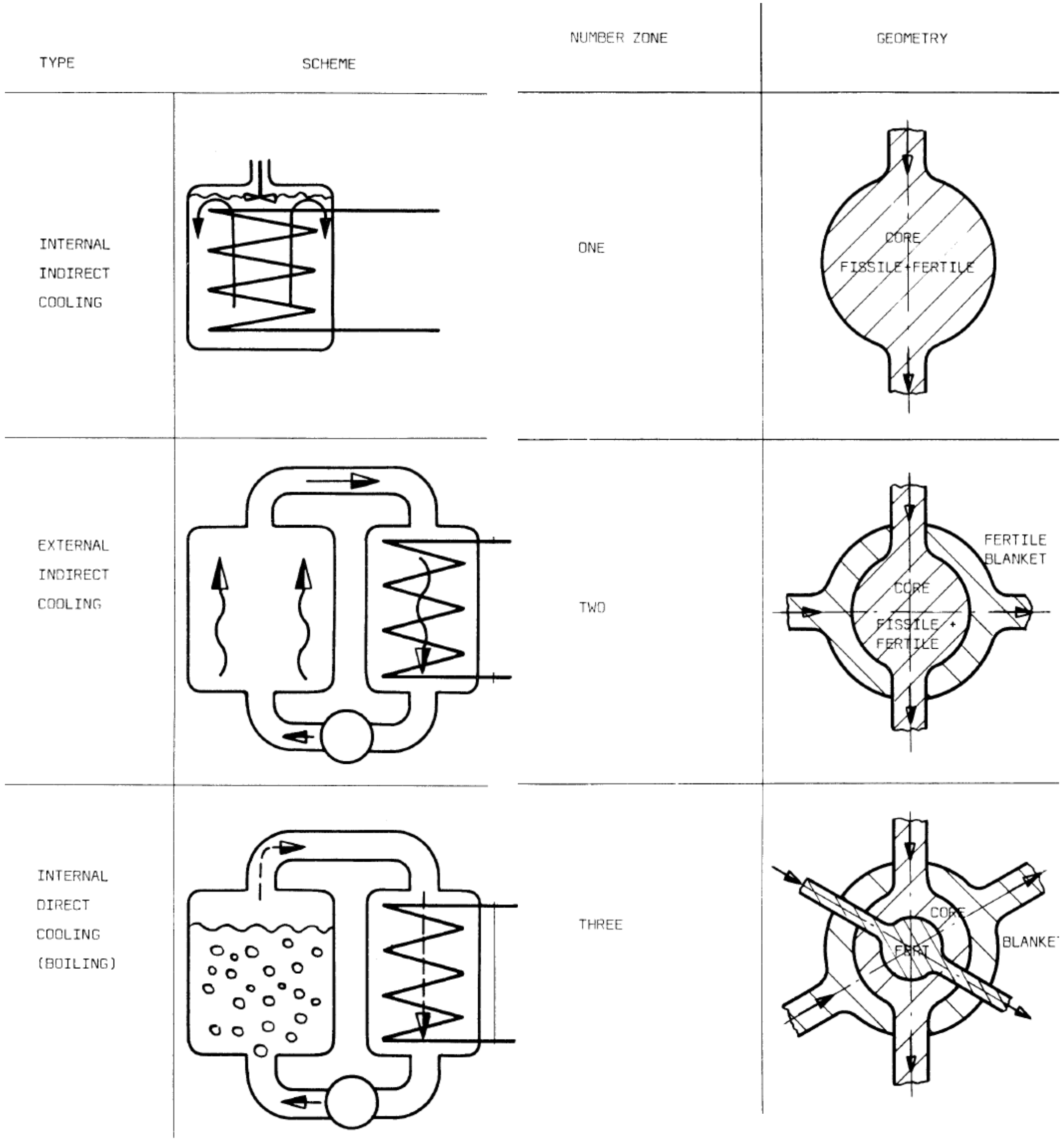
d) Kind of fissile nuclides and fuel cycles

e) Neutron energy

f) Purpose of the reactor

g) Dilutent for the molten salt

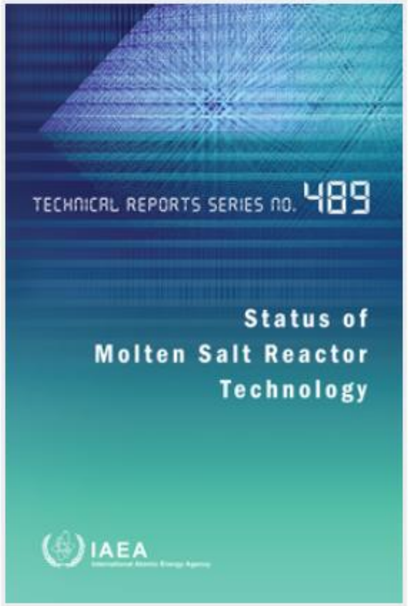
It is clear that such an arbitrary classification is not necessarily internally compatible and not all reactor types fall easily into the scheme chosen.



TAUBE, M., Fast Reactors Using Molten Chloride Salts as Fuel — Final Report (1972–1977), Rep. EIR-332, Eidg. Institut für Reaktorforschung, Würenlingen, Switzerland (1978).

MSR Taxonomy from the IAEA TRS No. 489

Status of Molten Salt Reactor Technology



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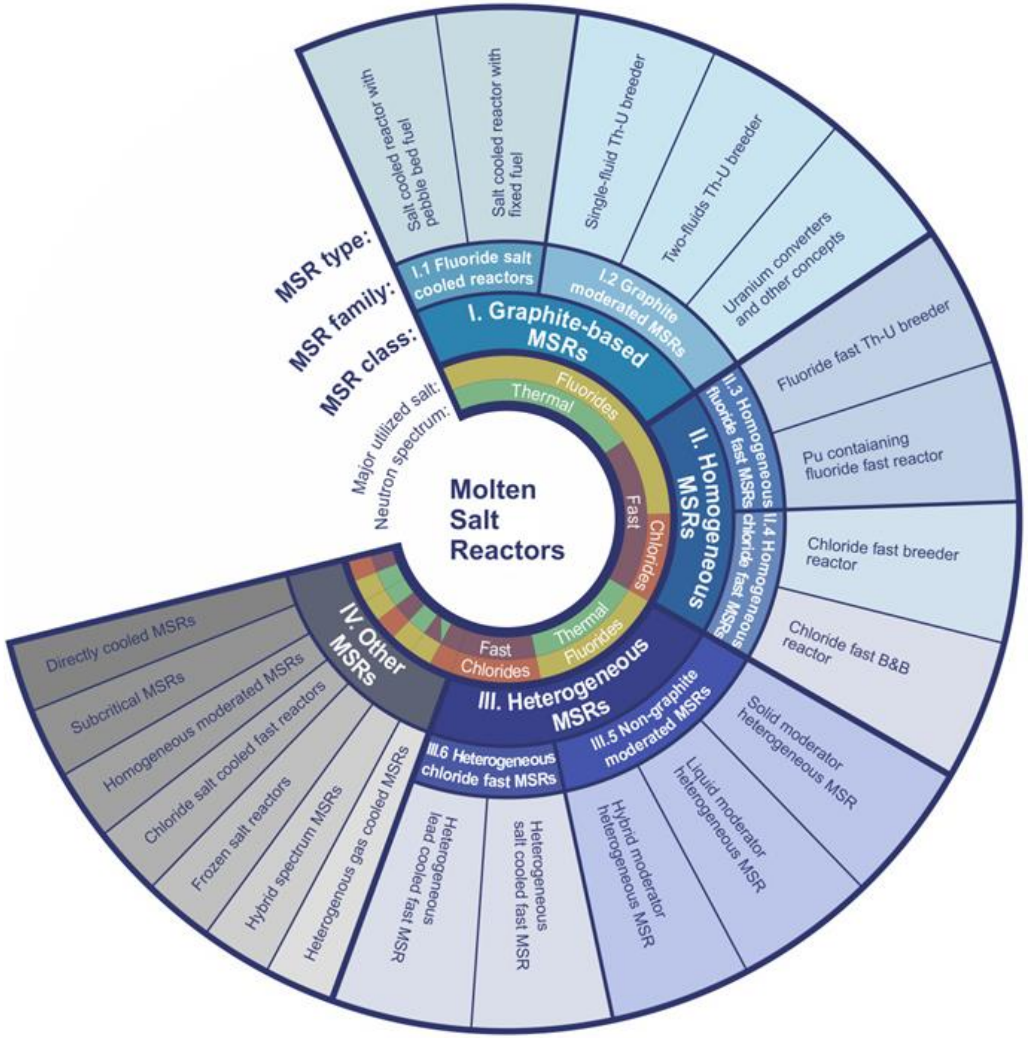
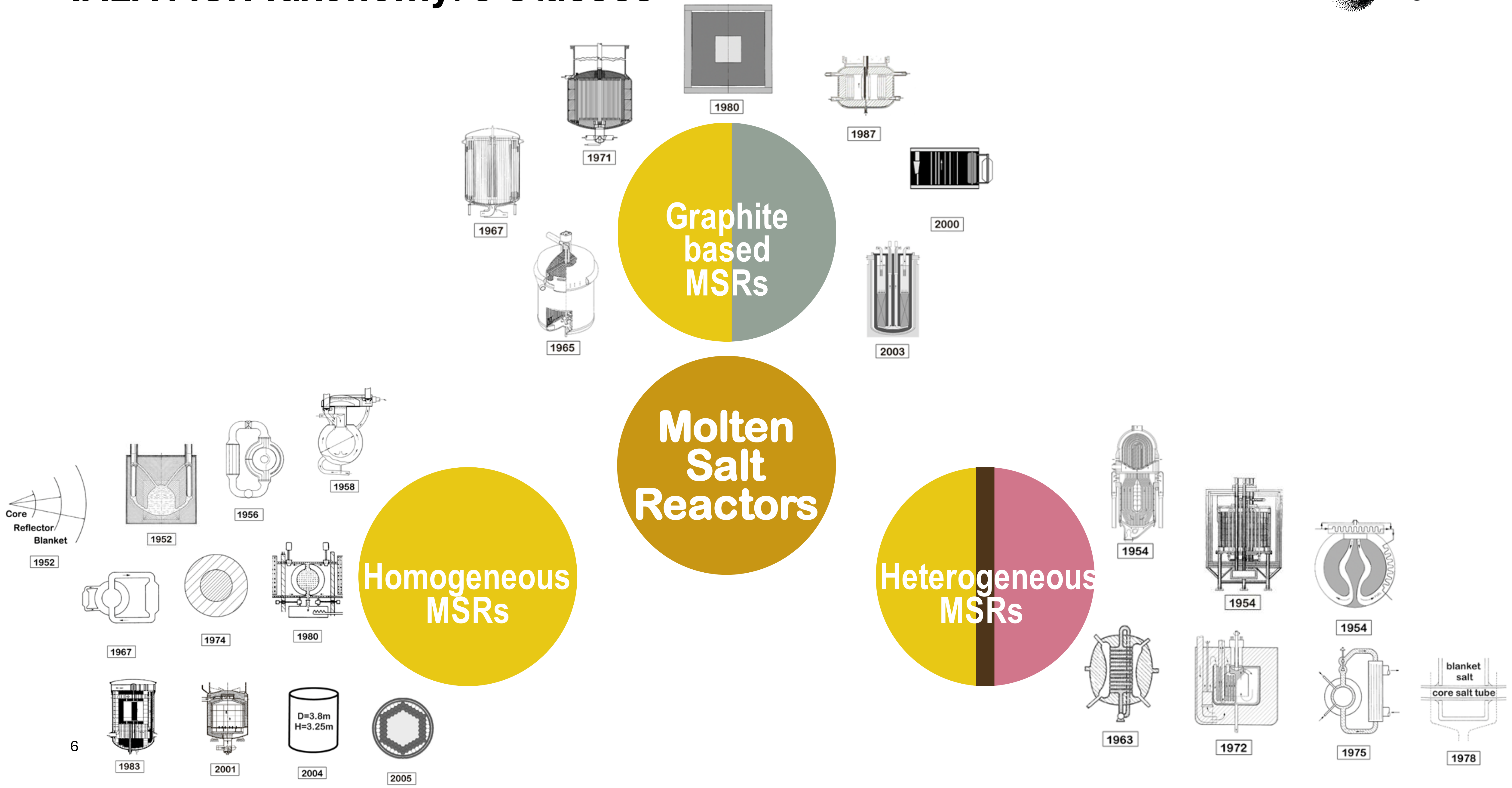
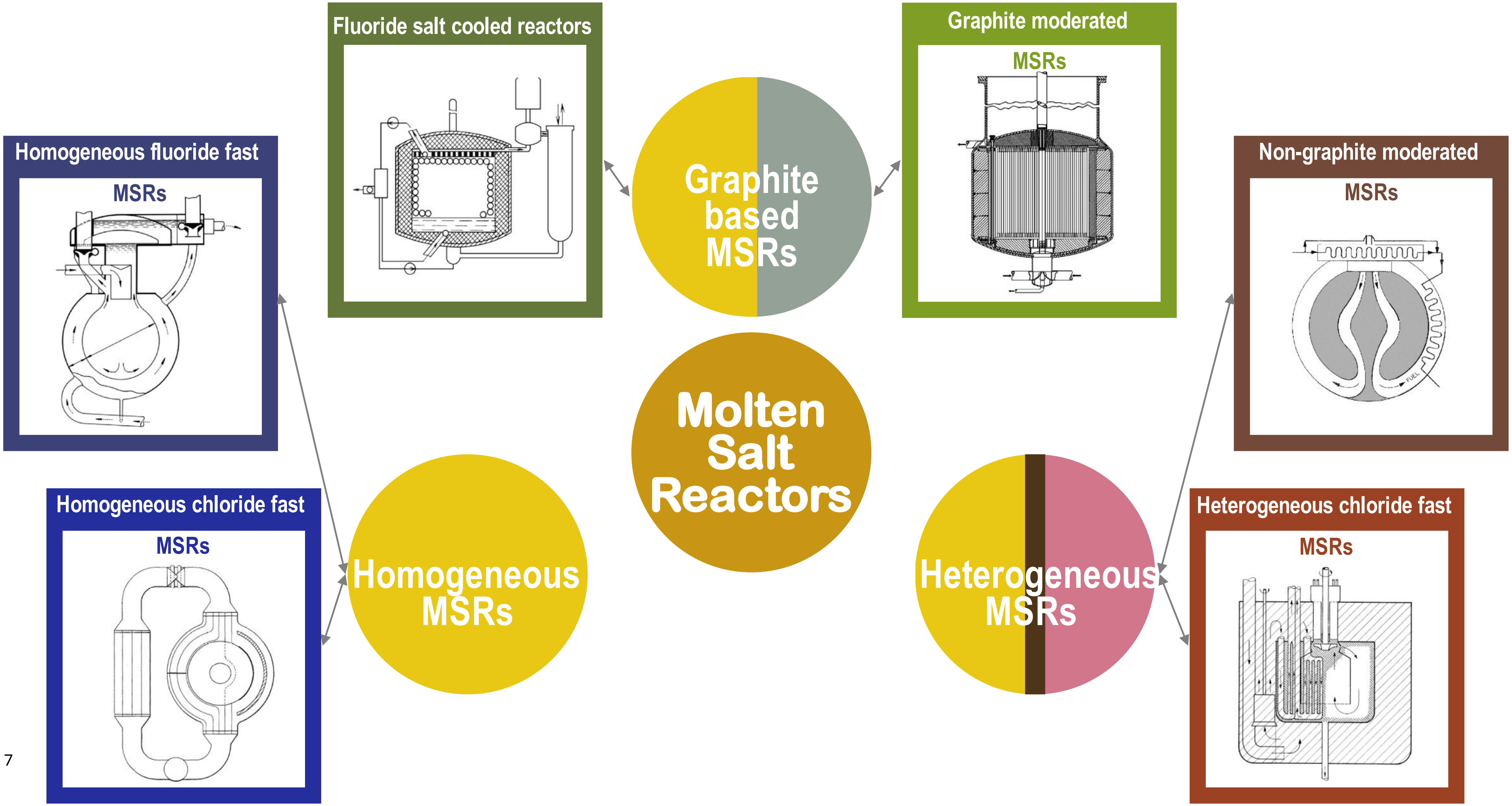


https://www.iaea.org/publications/14998/status-of-molten-salt-reactor-technology

IAEA MSR Taxonomy: 3 Classes



IAEA MSR Taxonomy: 6 Families



IAEA MSR Taxonomy: basic features

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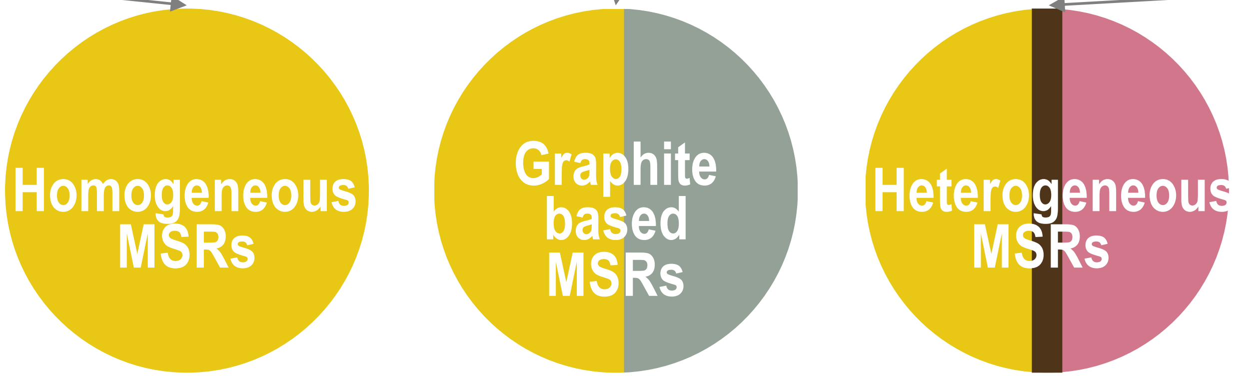
- Fluoride or Chloride salts acting as fuel and coolant.
- Fast spectrum *(epithermal with Be)*
- Chlorides: U-Pu, hard spectrum, transparent for neutrons.
- Fluorides: Th-U, softer spectrum, scattering neutrons.
- F and Cl mixture or other salts/halides usually not considered.
- Regular vessel replacement.

- Fluoride salt. *(high Cl neutron captures)*
- Possibility of Th-U cycle. *(demanding, fast fuel cleaning needed)*
- LEU fuel cycle.
- In case of solid fuel embedded in graphite, only moderating salts, like LiF-BeF_2, provides negative density effect.
- Regular graphite replacement.

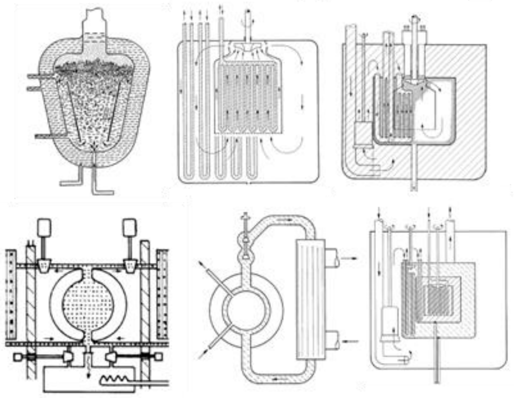
- Parasitic neutron capture of separating material. *(composites?)*
- Material choice determines breeding capability.
- Fluoride salt for moderated systems. *(high Cl neutron captures)*
- Chloride salts for fast systems. *(reactivity excess needed)*
- In case of two liquids, cooling can be distributed.
- Regular structural material replacement.



History of MSR research at PSI (EIR)

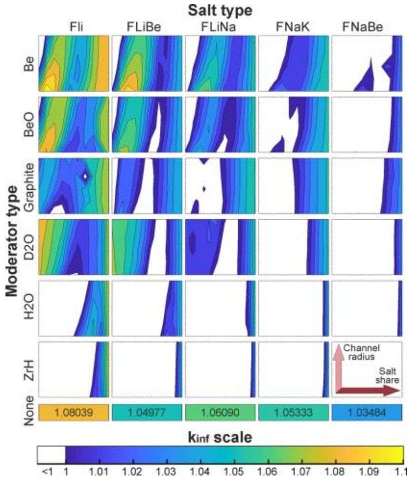
1970s -1980s EIR

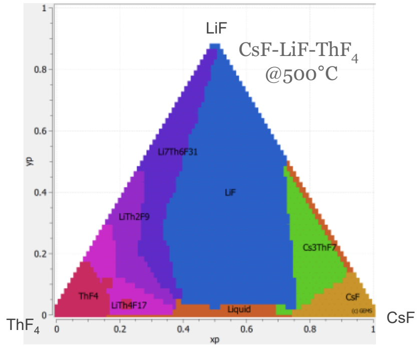
- MSR research was lead by Prof. Taube, several chloride based concepts (breeders and/or dedicated transmutors) have been accessed.



2012 – present PSI

- In **2012** the Advanced Nuclear System group included MSR as one of the monitored Gen-IV system of interest and joined the EU projects:
  EVOL *(2010-2013, observer)*, **SAMOFAR** *(2015-2019)*, **SAMOSAFER** *(2019-2023)*
- In **2014** a PhD project dedicated to MSR was financed by **SNSF**; major highlight:
  development of EQL0D fuel cycle procedure and
  identification of breed-and-burn fuel cycle capability in chloride fast MSR.
- Since **2015** Switzerland represented by PSI participate on the **Gen-IV MSR** project.
  (*act as a chair now*).
- In **2023** scoping study dedicated to transmutation capability encompassing MSR reactors was financed by **SNSF**.
- In the fall **2024** the 4th consecutive EU MSR project **ENDURANCE** (*2024-2028*) started with strong PSI and also ETHZ contributions.
- It resulted in more than **20** MSc, PhD, and visiting PhD theses with PSI involvement.





List of accomplished MSc and PhD theses

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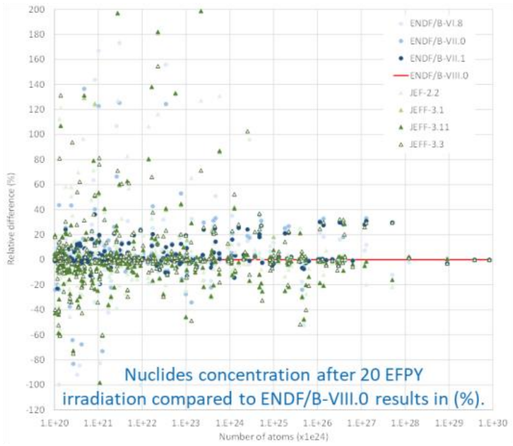
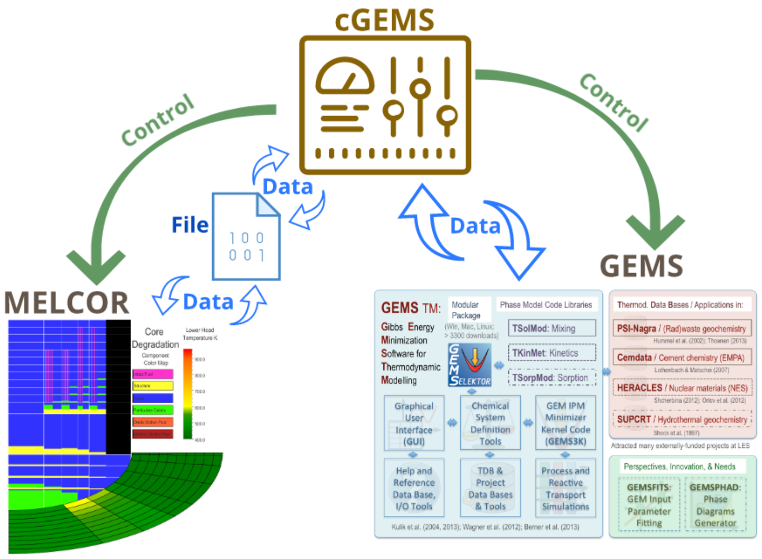
- Listed are also several theses accomplished in cooperation with other institutes or by visiting students from PoliMi and CTU Prague.

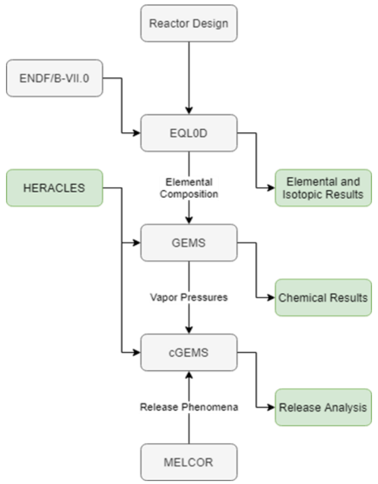
Name	Title	Thesis type / Status	Year
B. Hombourger	Parametric Lattice Study for Conception of a Molten Salt Reactor in Closed Thorium Fuel Cycle	Swiss nuclear MSc course / Defended	2013
C. Fiorina	The Molten Salt Fast Reactor as a Fast-Spectrum Candidate for Thorium Implementation	PhD thesis in cooperation with PSI / Defended at POLIMI	2013
V. Ariu	Heat exchanger analysis for innovative molten salt fast reactor	Swiss MSc course / Defended	2014
M. Aufiero	Development of advanced simulation tools for circulating-fuel nuclear reactors	PhD thesis in cooperation with PSI / Defended at POLIMI	2014
H. Kim	Static and transient analysis of Molten Salt Reactor Experiment using SERPENT-2 / TRACE / PARCS codes	Swiss nuclear MSc course / Defended	2015
J. Choe	Empirical Decay Heat Correlations and Fission Products Behavior in MSRs	Swiss nuclear MSc course / Defended	2015
J. Bao	Development of the model for the multiphysics analysis of Molten Salt Reactor Experiment using GeN-Foam code	Swiss nuclear MSc course / Defended	2016
D. Pyron	Safety Analysis for the Licensing of Molten Salt Reactors	Swiss nuclear MSc course / Defended	2016
E. Pettersen	Coupled multi-physics simulations of the MSFR using TRACE-PARCS	MSc thesis in cooperation with PSI / Defended at Univ. Paris-Saclay	2016
N. Vozarova	Behaviour of fission products in the molten salt reactor fuel	Swiss MSc course in cooperation with JRC Karlsruhe / Defended at ETHZ	2016
M. Zanneti	Development of new tools for the analysis and simulation of circulating-fuel reactor power plants	PhD thesis in cooperation with PSI / Defended at POLIMI	2016
E. Losa	U-Pu and Th-U Fuel Cycle Closure	PhD thesis in cooperation with PSI / Defended at TU Prague	2017
B. Hombourger	Small modular Molten Salt Fast Reactor design for closed fuel cycle	PhD thesis in frame of SNSF project at PSI Defended at EPFL	2018
M. Di Filippo	Development of dedicated MSR burn-up tool	Swiss nuclear MSc course / Defended	2018
V. Sisl	Thorium Utilization in the Fuel Cycle of Advanced Nuclear Reactors	MSc thesis in cooperation with PSI / Defended at TU Prague	2018
T. Koivisto	Assessment of waste burning in open cycle of two fluids chloride MSR	MSc thesis in cooperation with PSI / defended at Aalto University in Finland	2019
V. Raffuzzi	Modelling of batch-wise operation of European Sodium Fast Reactor and Breed&Burn Molten Salt Reactor	Swiss nuclear MSc course / Defended	2019
J. Dietz	Chemical-Thermodynamic Modelling of the MSR-Related Systems Under Normal and Accident Conditions	Swiss nuclear MSc course / Defended	2020
R. Gonzales	Improved methodology for analysis and design of Molten Salt Reactors	PhD thesis in frame of H2020 project SAMOFAR / Defended at EPFL	2021
J. Santora	Two-fluid Breed & Burn MCFR parametric study	Swiss nuclear MSc course / Defended	2022
F. Borys	Identification and evaluation of transmutation criteria for selected reactors	Swiss nuclear MSc course	2023
M. Krstovic	Extended Point Kinetics Solver For MSR	Swiss nuclear MSc course	2023

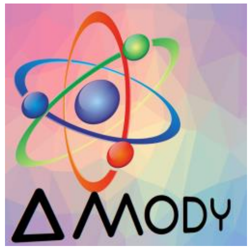
Major tools/competences

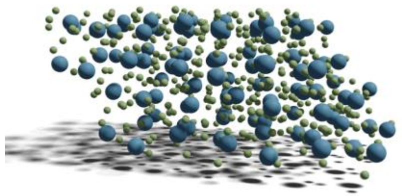
- **EQL0D & EQL3D**
  equilibrium cycle procedures.
- **TRACE-PARCS**
  system code for MSR transient analysis.
- **GeN-Foam / Atari**
  multi-physics tools for MSR core analysis.
- **GEMS**
  Gibbs Energy Minimization Software.
- **cGEMS**
  (GEMS-MELCOR) coupling for
  severe accidents simulation.
- **AMoDy**
  Molecular dynamics tool.

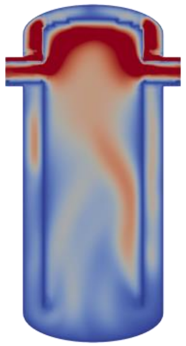


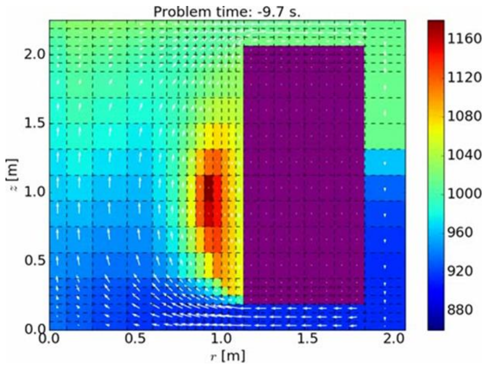


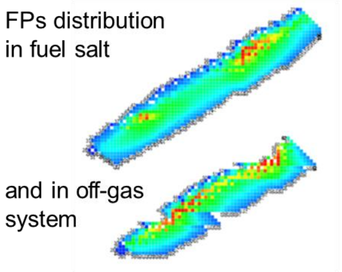






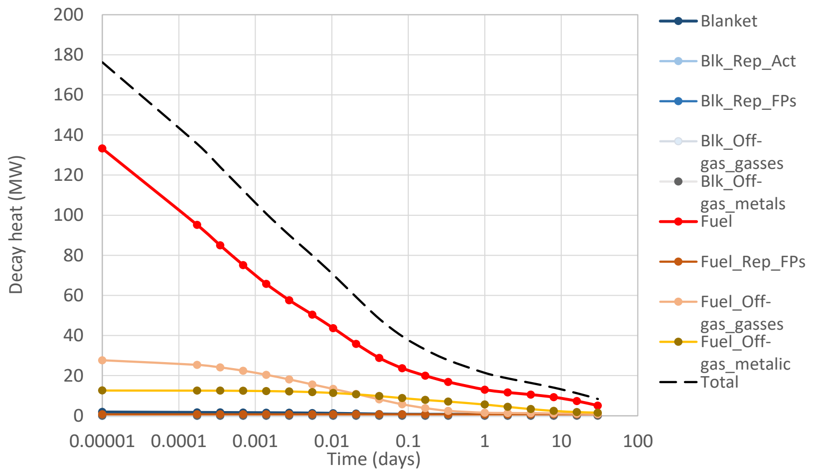






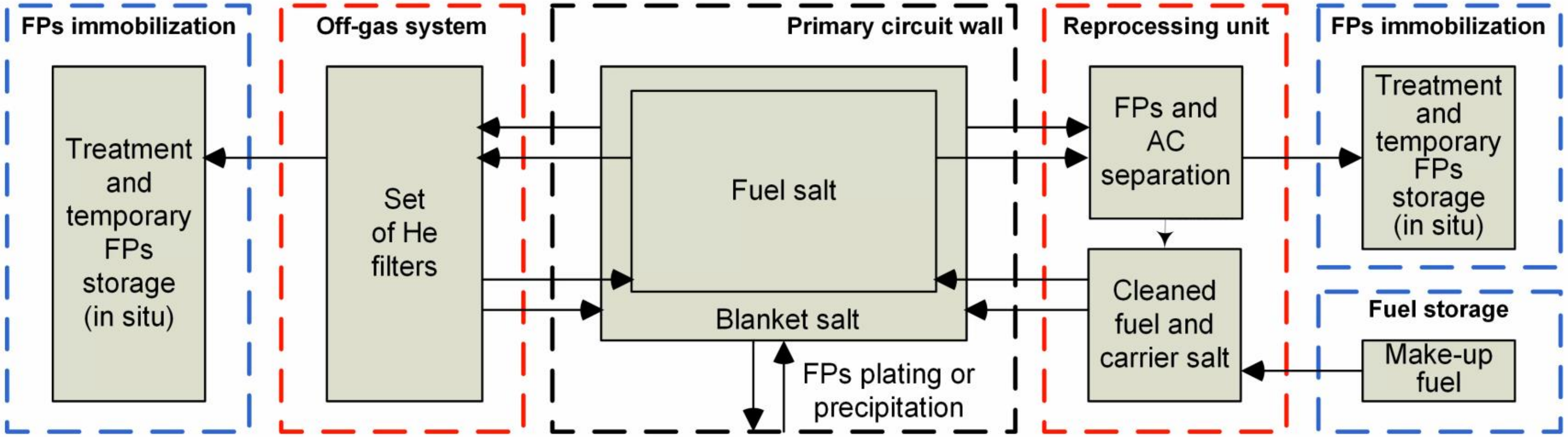
EQL0D simulations: Distributed source term

- Development of dedicated EQL0D burnup tool for liquid reactors.
- Benchmark proposal for fuel cycle burnup tools.
- Radiotoxicity and decay heat distribution simulation in different locations of the system:
  1. core,
  2. blanket,
  3. off gas,
  4. reprocessing unit...



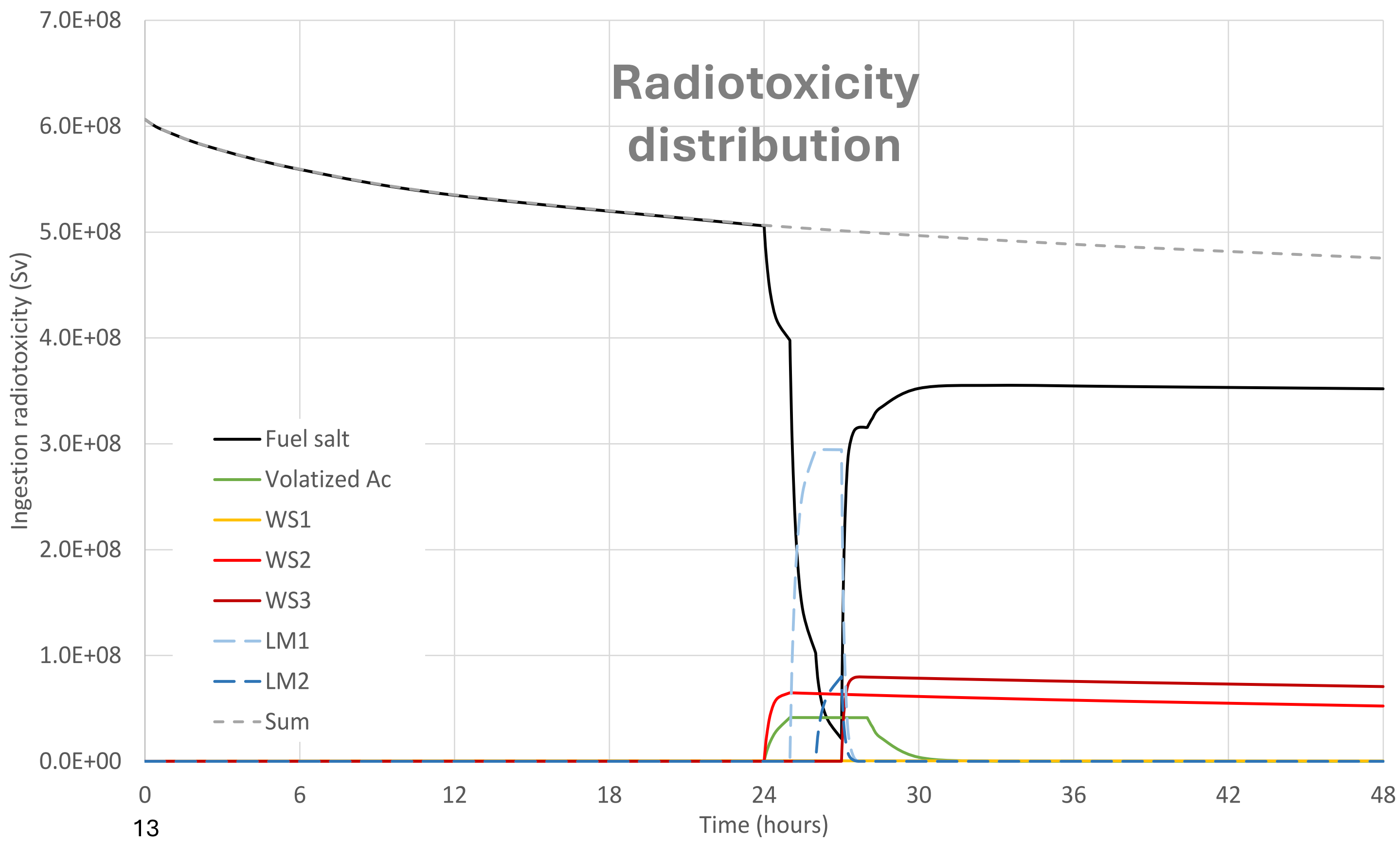
Decay heat distribution

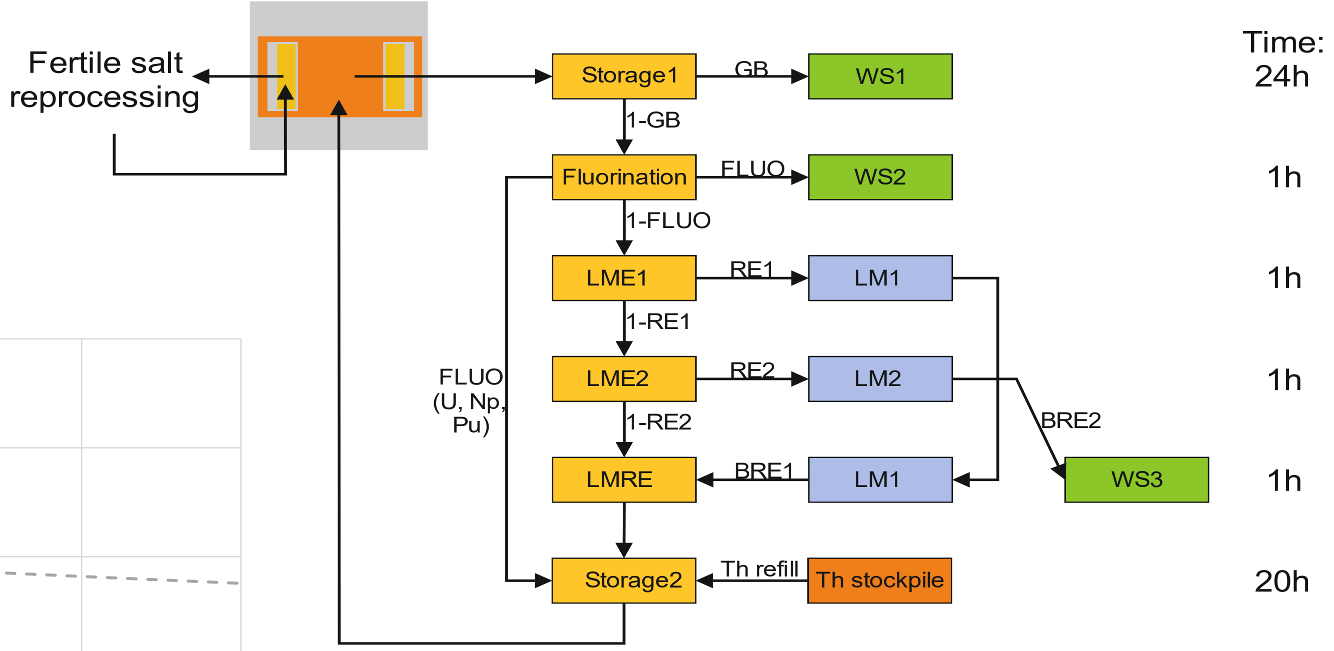
Different locations of fission products in Molten Salt Fast Reactor



EQL0D simulations: Reprocessing unit

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





Locations of reprocessing unit in typical MSR

Core size comparison for closed and open B&B cycle

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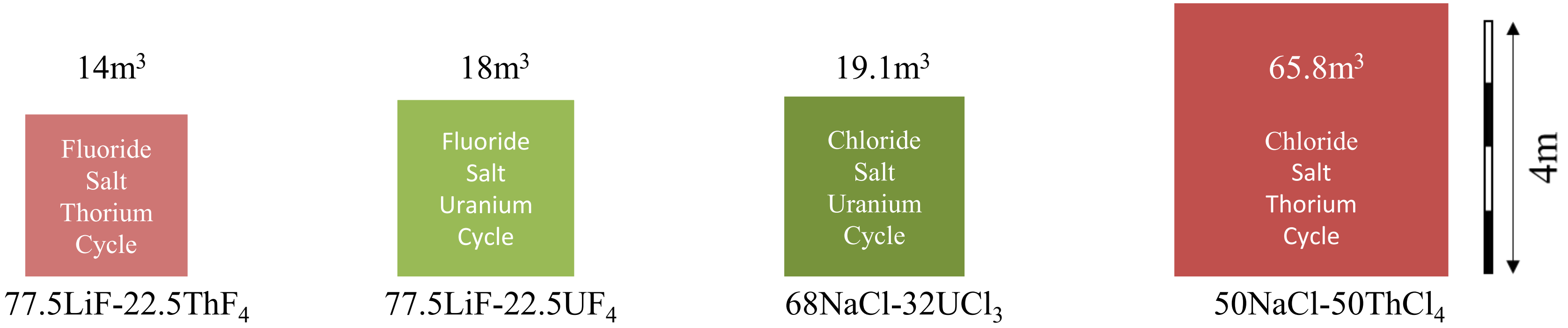
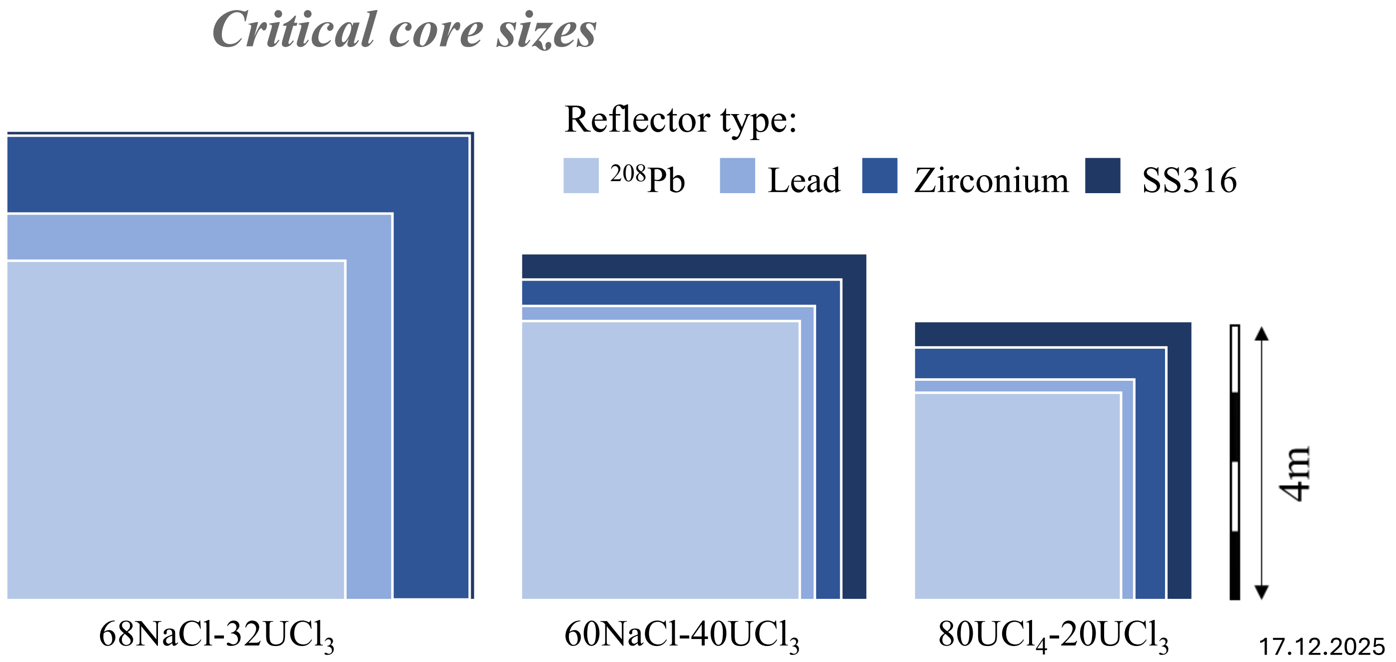
- Closed cycle



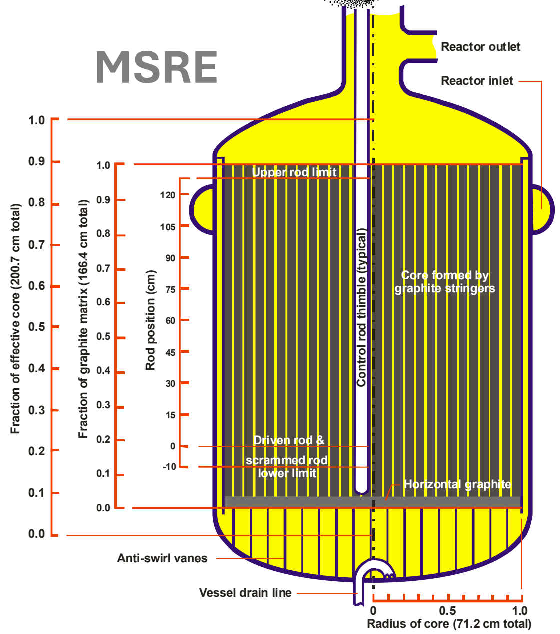
- Breed and burn open cycle



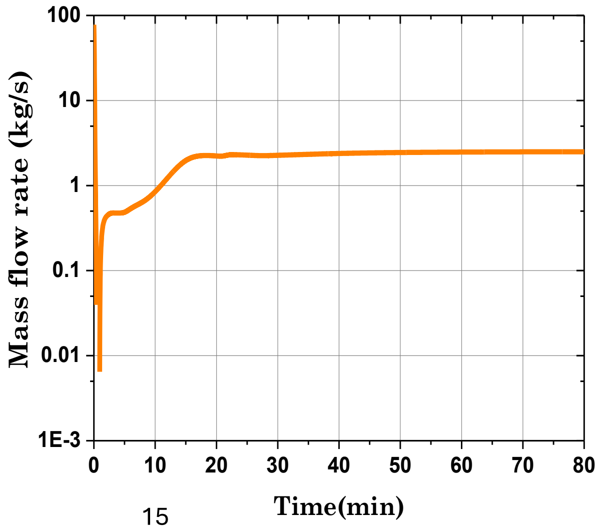
Hombourger, B.A., 2018. Ph.D. Thesis. EPFL Lausanne, Switzerland.

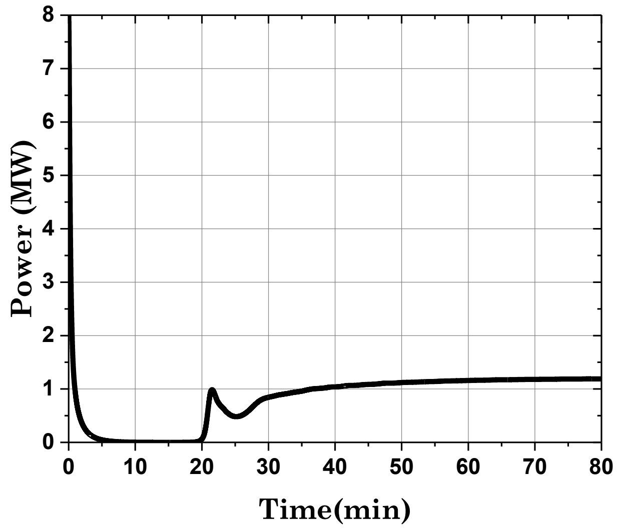
TRACE application to MSRE

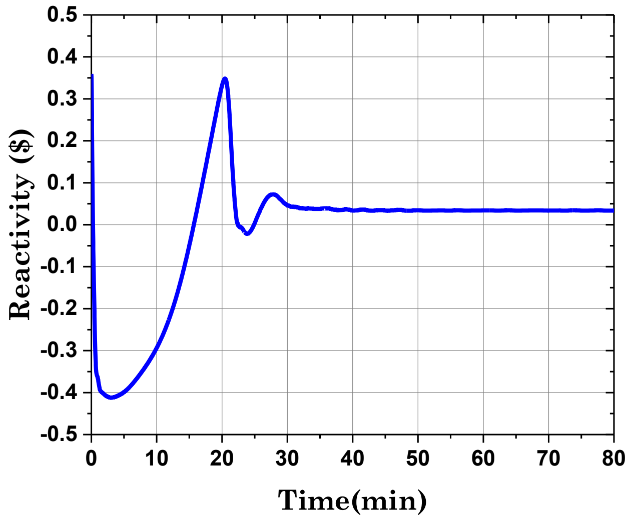
- **TRACE-PARCS** system code application to **MSRE**.
- Individuation and preliminary assessment of major accidental transients or optimization of the design.
- Unprotected pump trip as example result.
  - Initial overheating stops the chain reaction.
  - Natural circulation leads later to stabilized power level.

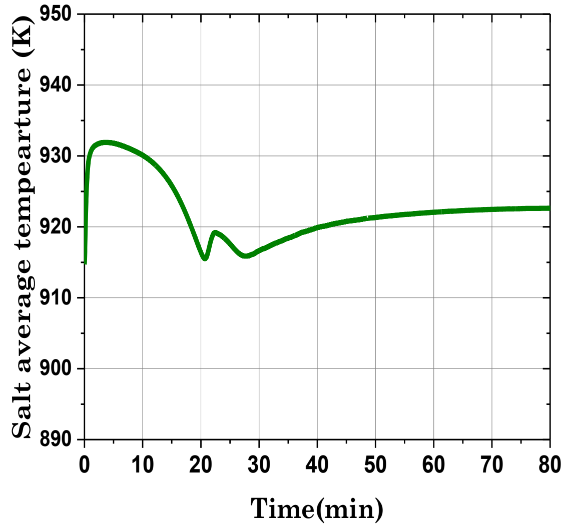


H. Kim, LRS, MSc thesis 2015





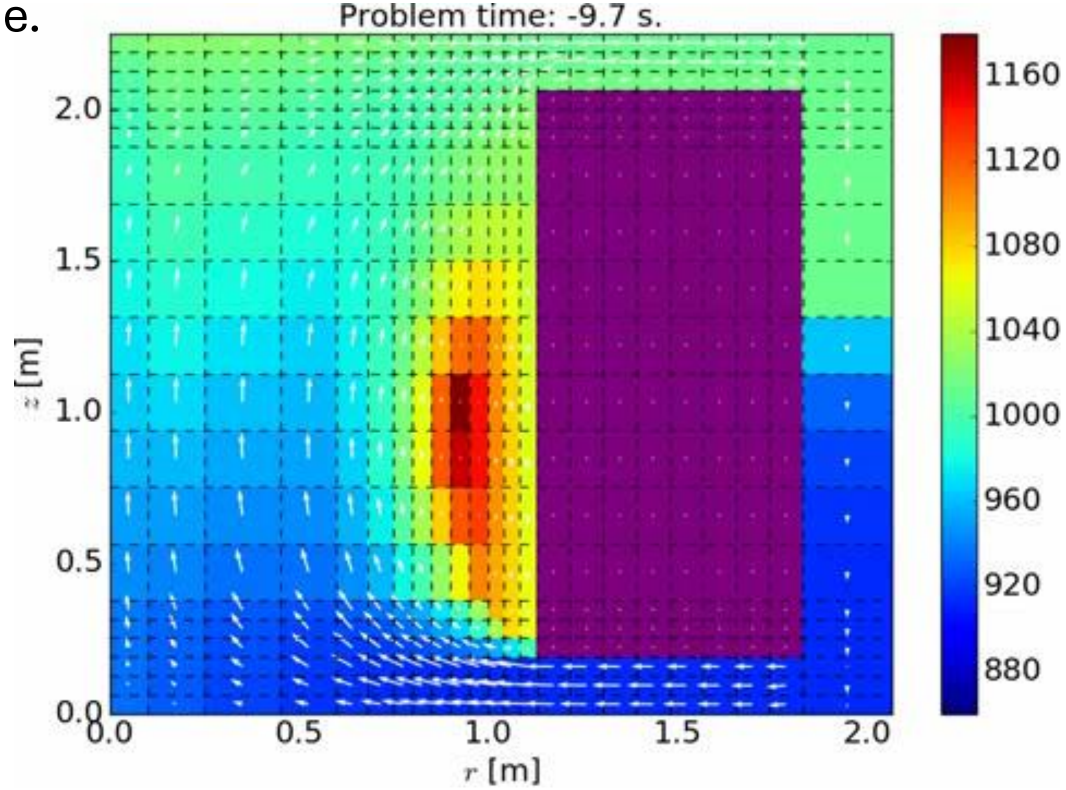




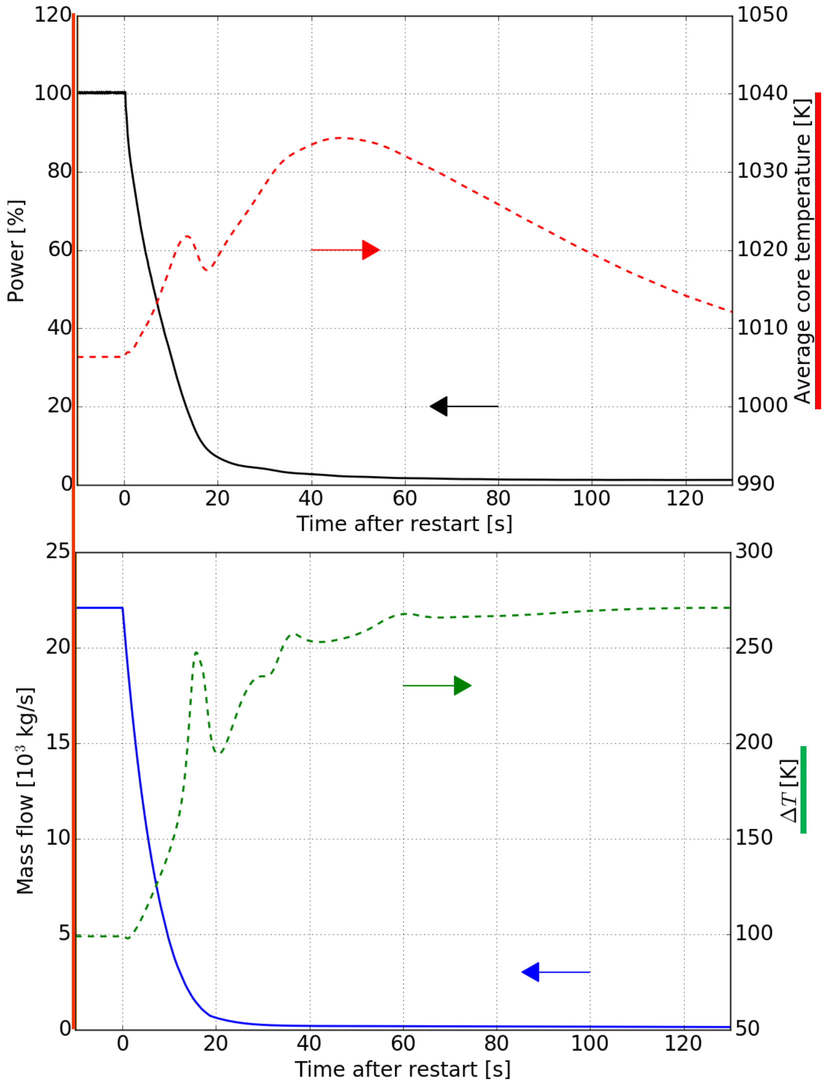
Zanetti, M., et al., Extension of the fast code system for the modeling and simulation of MSR dynamics Proceedings of ICAPP 2015.

TRACE application to MSFR

- **TRACE-PARCS** system code application to **MSFR**.
- Applying TRACE vessel component.
- Applicable for 3D transients (2D symmetric transients).
- Capability of system analysis with acceptable accuracy and CPU time.



E. Pettersen, LRS, MSc thesis 2016

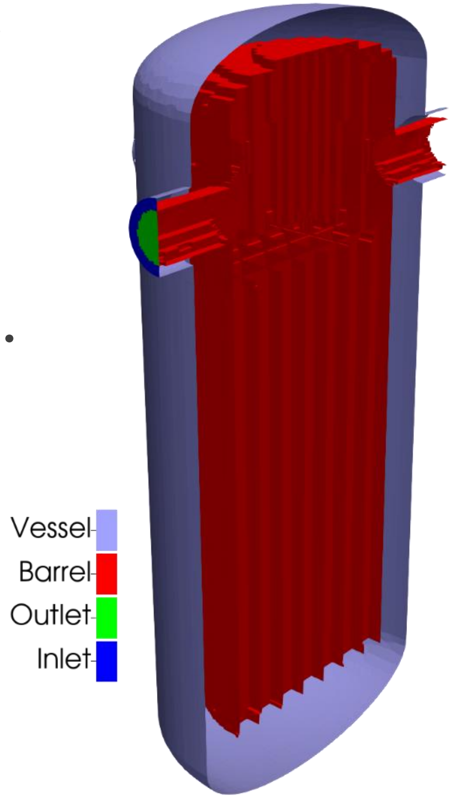


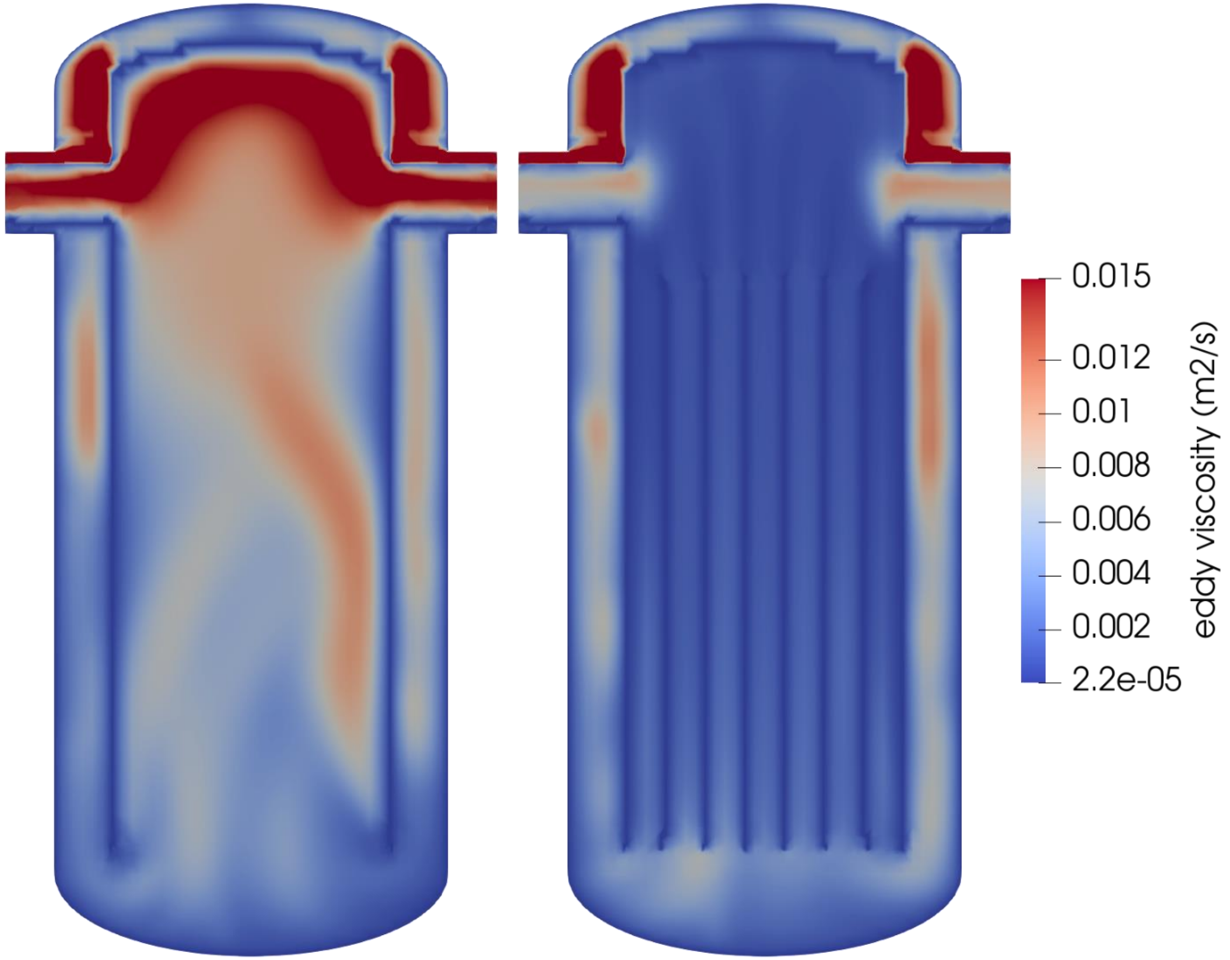
ULOF- unprotected loss of flow

Atari code: application to MCFR "Tap" reactor

- Atari code was also applied to a large MCFR concept with HDR of 2:1.
- The baffles for flow direction control were accessed.
- Their need is not obvious.

Power	3 GW
Salt volume	200 m^3
Composition	60-40 $NaCl\text{-}UCl_3$
Reflector	PbO
Height	11.6 m
Diameter	4.8 m



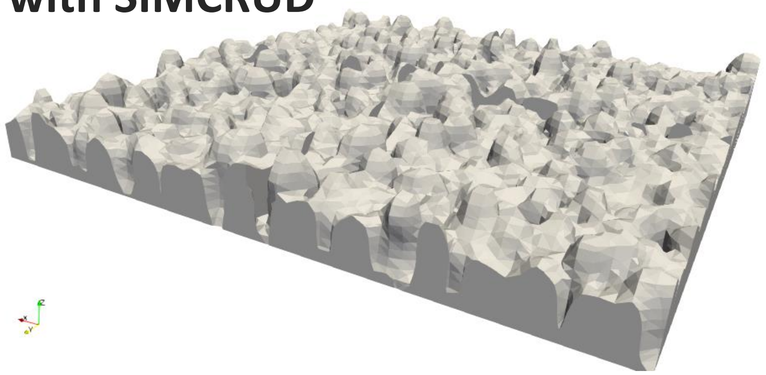


DE OLIVEIRA, R.G.G., HOMBOURGER, B.A., Fuel tap: a simplified breed-and-burn MSR, (Proc. Physics of Reactors (PHYSOR) 2020, Cambridge, United Kingdom), (2020).

GEMS code with Heracles database

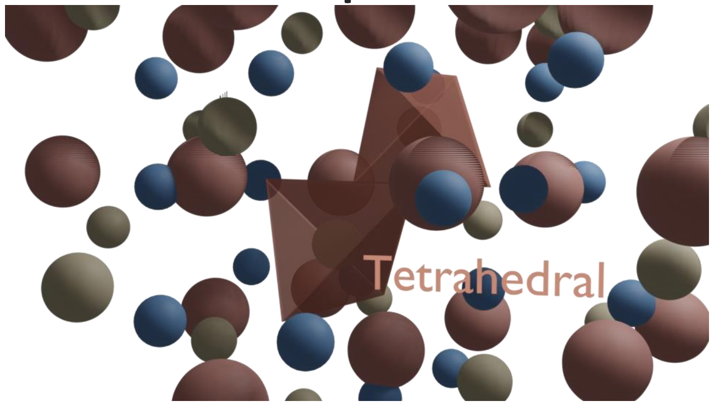
ETH zürich PSI

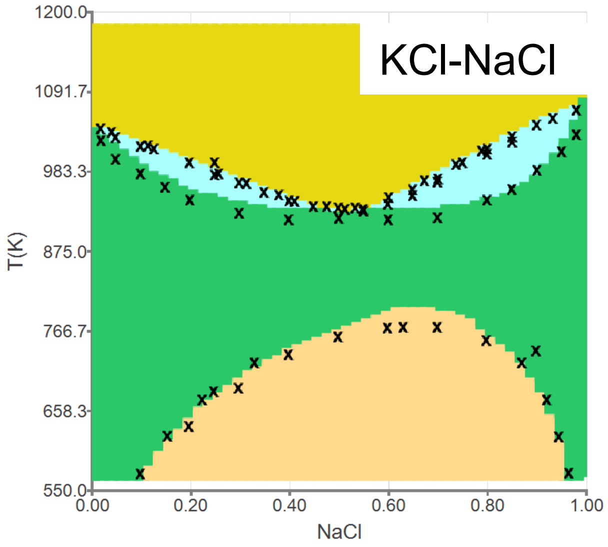
Aqueous chemistry (e.g. CRUDS formation) with SIMCRUD



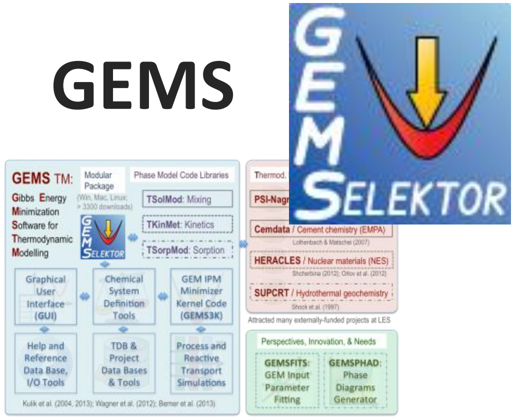
- aqueous electrolyte;
- non-ideal gaseous fluids;
- non-ideal solid solutions;
- non-ideal (ionic) melts;
- adsorption, ion exchange;
- metastable species / phases, kinetics
- ≈30 different mixing models

Inversion in spinel structure

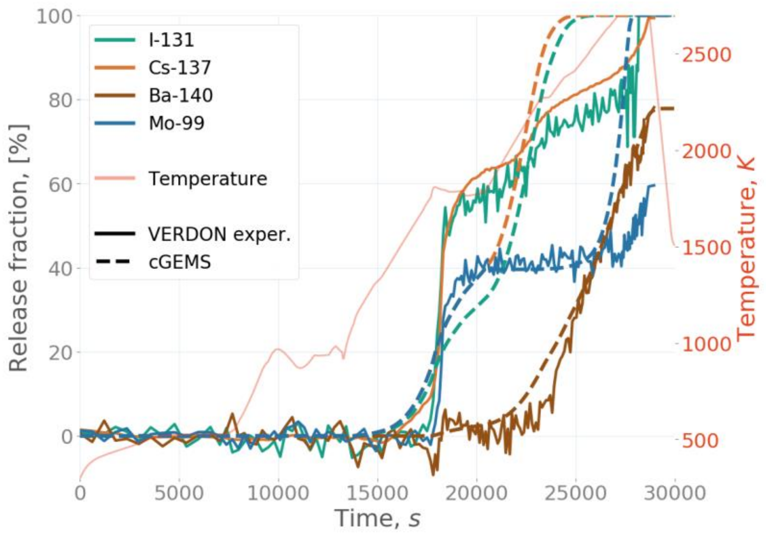




GEMS



FP Release (e.g. SA related problems) with cGEMS

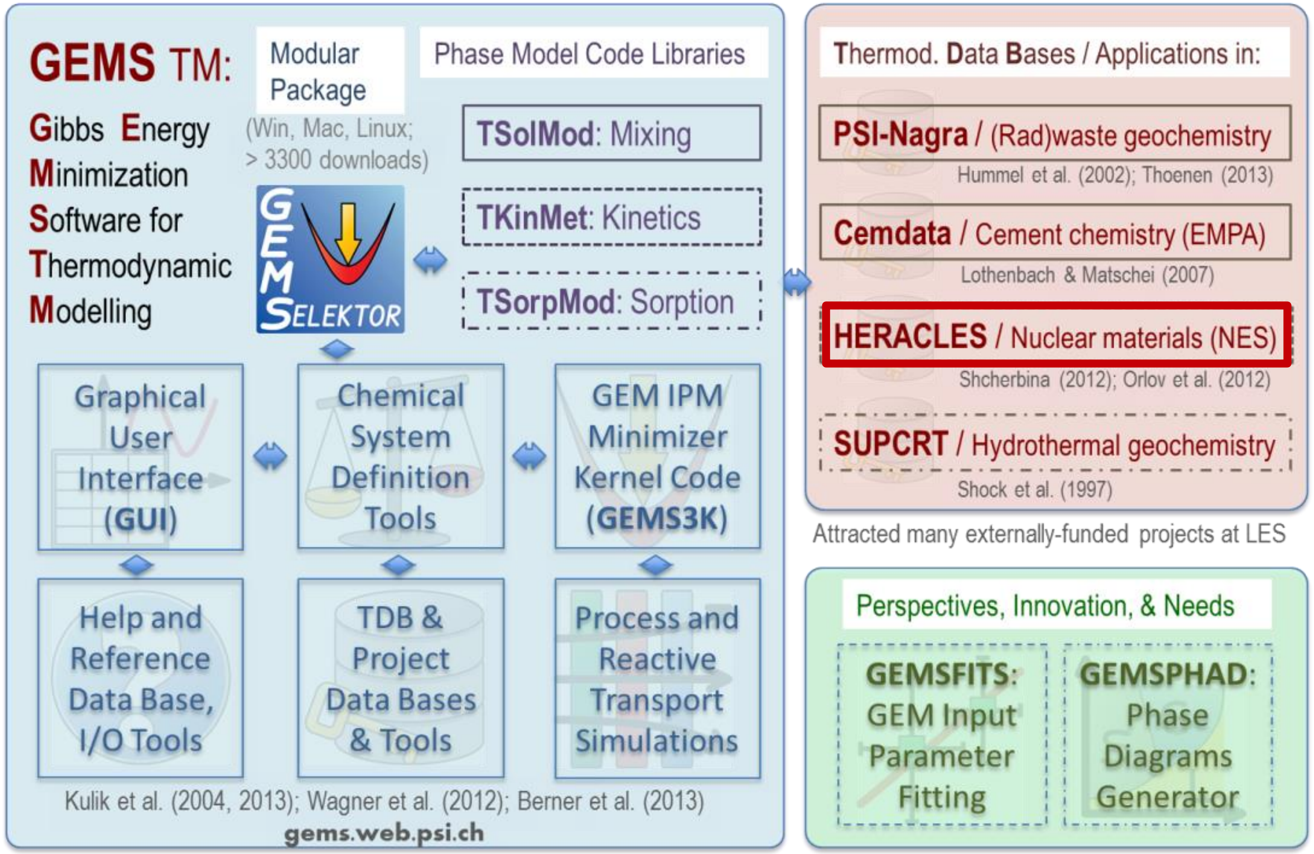


GEMS code with Heracles database

- PSI has a competence in thermodynamics simulations. In-house code GEMS (Gibbs Energy Minimization Software) is unique open source alternative to the commercial FactSage code.

- The respective HERACLES database and selected models were extended or modified.

- Proper phase diagram plotter is still missing.



homepage http://gems.web.psi.ch

Kulik D.A., Dmytrieva S.V., Wagner T., Kosakowski G., Thoenen T, Berner U., et al. (2004-2014): Gibbs Energy Minimization Software (GEMS)

Recent update of GEMS Heracles database

ETH zürich PSI

Current list of species:

150 chloride species, 1170 total number of species in HERACLES DB, ~50% applicable for MSR

Gaseous species

AlCl(g)	KCl(g)	SeF5Cl(g)	ZrCl2(g)
BaCl(g)	KI(g)	SeOCl2(g)	ZrCl3(g)
BaCl2(g)	LaCl3(g)	SnCl(g)	ZrCl4(g)
BiCl(g)	Li2Cl2(g)	SnCl2(g)	
BiCl3(g)	LiCl(g)	SnCl3(g)	
BrCl(g)	LiClO(g)	SrCl(g)	
CaCl(g)	MgCl2(g)	SrCl2(g)	
CaCl2(g)	MoCl4(g)	TeCl2(g)	
CeCl3(g)	MoCl5(g)	TeCl4(g)	
Cl(g)	MoCl6(g)	ThCl2(g)	
Cl2(g)	NaCl(g)	ThCl3(g)	
Cl2O(g)	NaI(g)	ThCl4(g)	
ClO(g)	NdCl3(g)	UCl(g)	
ClO2(g)	NpCl3(g)	UCl2(g)	
Cs2Cl2(g)	NpCl4(g)	UCl3(g)	
CsCl(g)	PrCl3(g)	UCl4(g)	
HCl(g)	PuCl3(g)	UCl5(g)	
HOCl(g)	PuCl4(g)	UCl6(g)	
ICl(g)	Se2Cl2(g)	UO2Cl2(g)	
K2Cl2(g)	SeCl2(g)	ZrCl(g)	

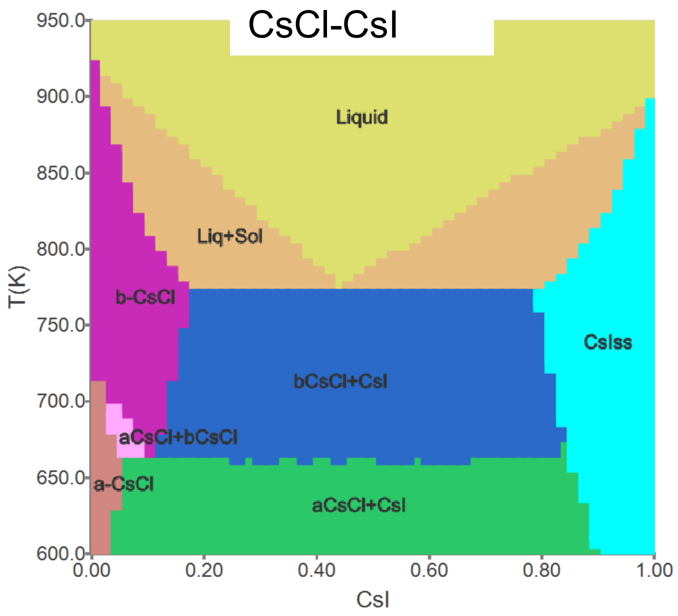
Liquid species

BaCl2(l)	RbCl(l)
BiCl3(l)	SnCl2(l)
CaCl2(l)	SnCl4(l)
CdCl2(l)	SrCl2(l)
CeCl3(l)	TeCl4(l)
CsCl(l)	ThCl4(l)
KCaCl3(l)	UCl3(l)
KCl(l)	UCl4(l)
KI(l)	ZrCl2(l)
LaCl3(l)	
LiCl(l)	
MgCl2(l)	
MoCl4(l)	
MoCl5(l)	
NaCl(l)	
NaI(l)	
NdCl3(l)	
NpCl4(l)	
PrCl3(l)	
PuCl3(l)	

Solid species

AmCl3	MoCl6	UCl3
AmOCl	NaCl(s)	UCl4
BaCl2	NaI	UCl5
BiCl3	Na2ThCl6	UCl6
BiOCl	NdCl3	UCl2F2
CaCl2	NpCl3	UCl3F
CdCl2	NpCl4	UClF3
CeCl3	NpOCl2	U2O2Cl5
CsCl	PrCl3	UO2Cl
Cs2PuCl6	PuCl3	UO2Cl2
Cs3PuCl6	PuOCl	UOCl
CsPu2Cl7	RbCl	UOCl2
KCaCl3	SeCl4	UOCl3
KCl	SnCl2	ZrCl
KI	SnCl4	ZrCl2
LaCl3	SrCl2	ZrCl3
LiCl	TeCl4	ZrCl4
MgCl2	ThCl2	
MoCl4	ThCl3	
MoCl5	ThCl4	

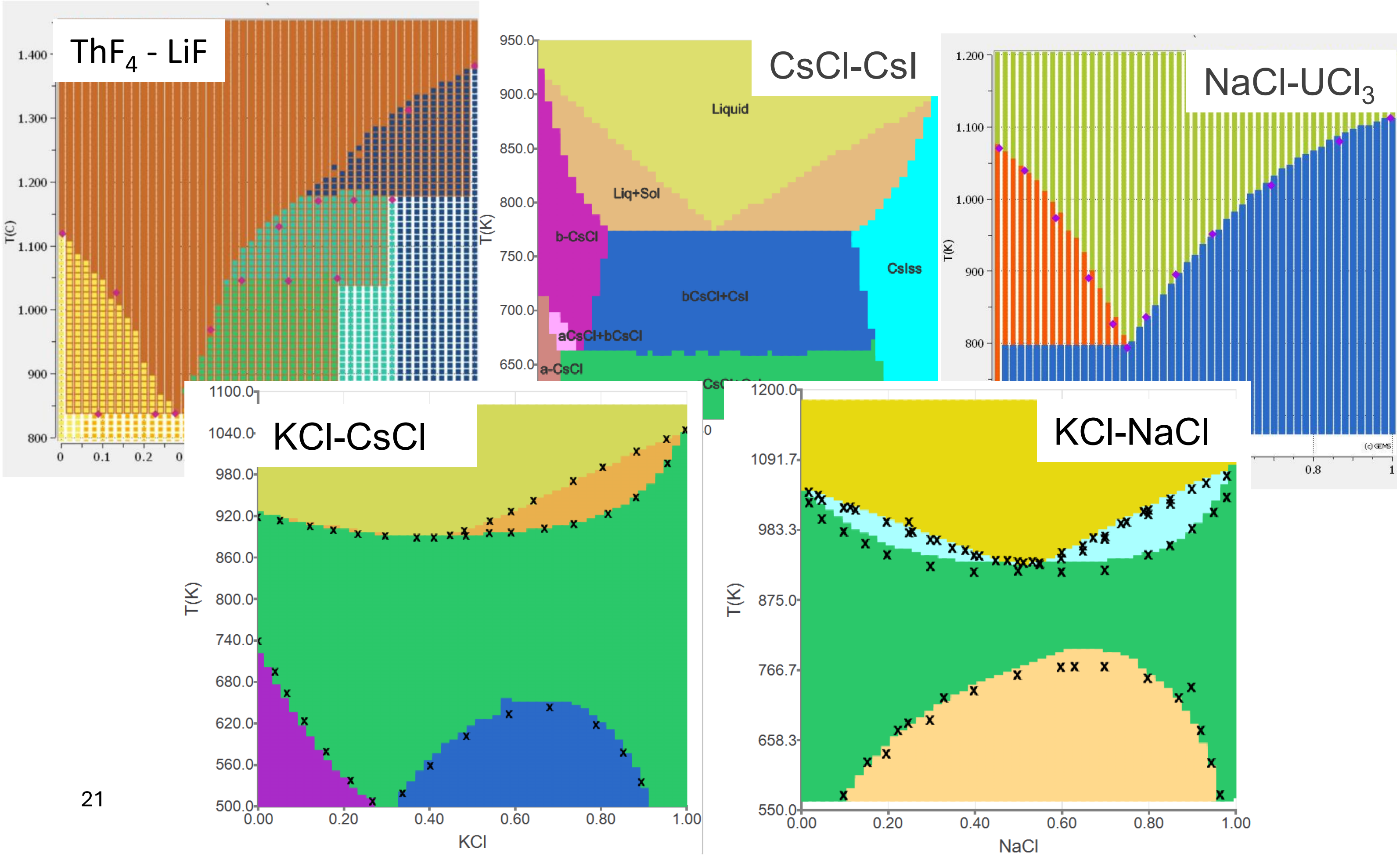
Page 5



Recent update of GEMS Heracles database

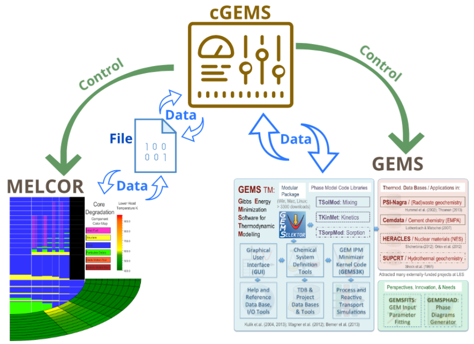
Optimized a number of binary diagrams:

$NaCl$-UCl_3, NaCl-PuCl3, PuCl3-UCl3, NaCl-ThCl4, CsCl-CsI, KCl-CsCl, KCl-NaCl, KCl-UCl3



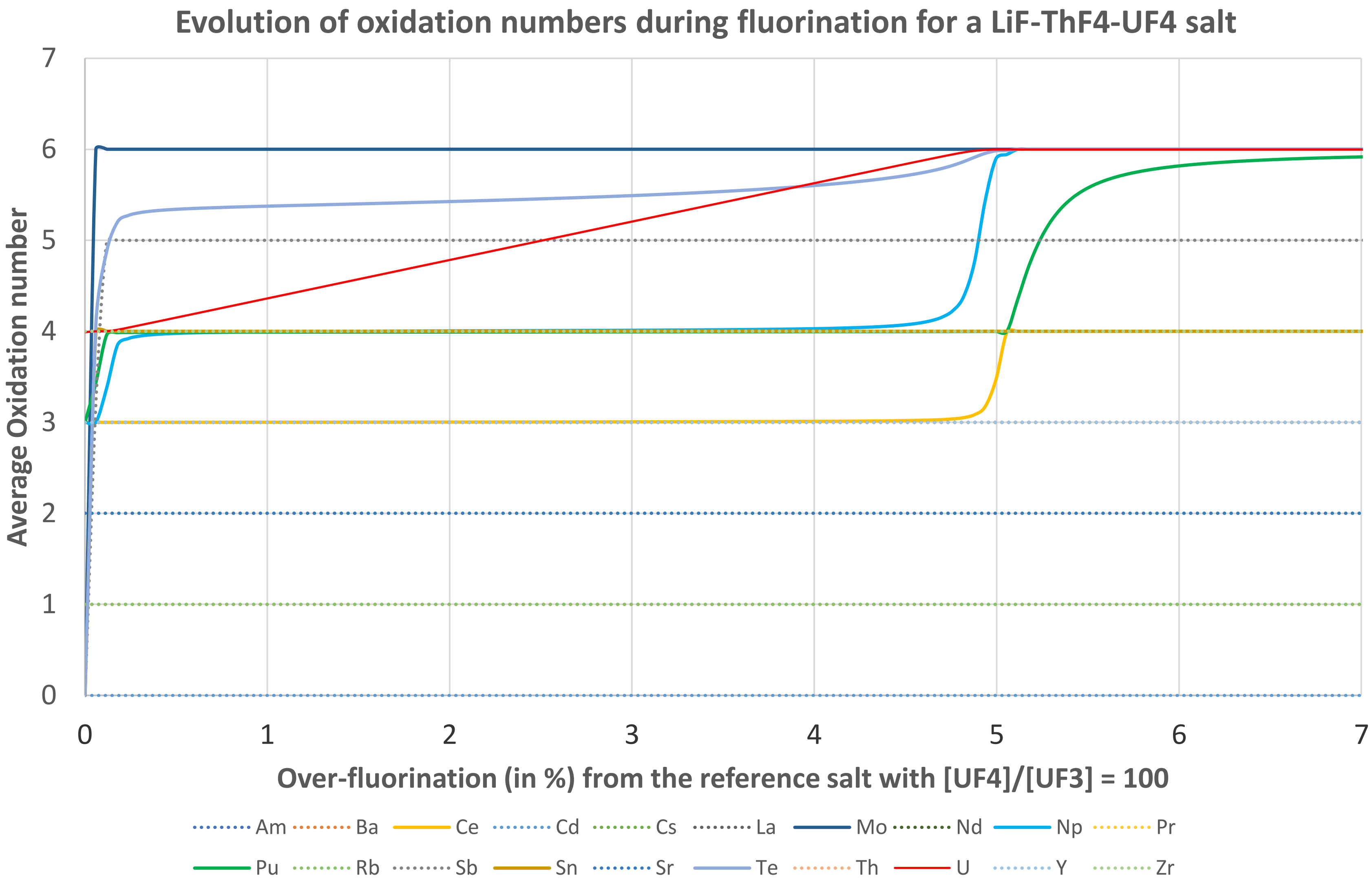
Develop a framework for modelling fission product release from a simulated molten salt pool for chloride- and fluoride-based systems.

Gain valuable insights into the chemical composition of salts within a molten salt pool and fission product release behaviour.



Redox window: volatilization

- Evolution of the oxidation number of the nuclides during fluorination

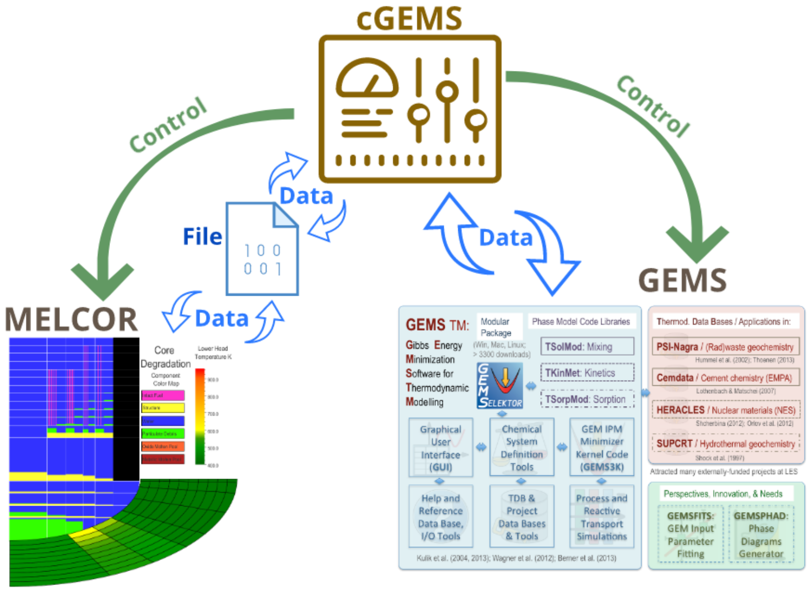


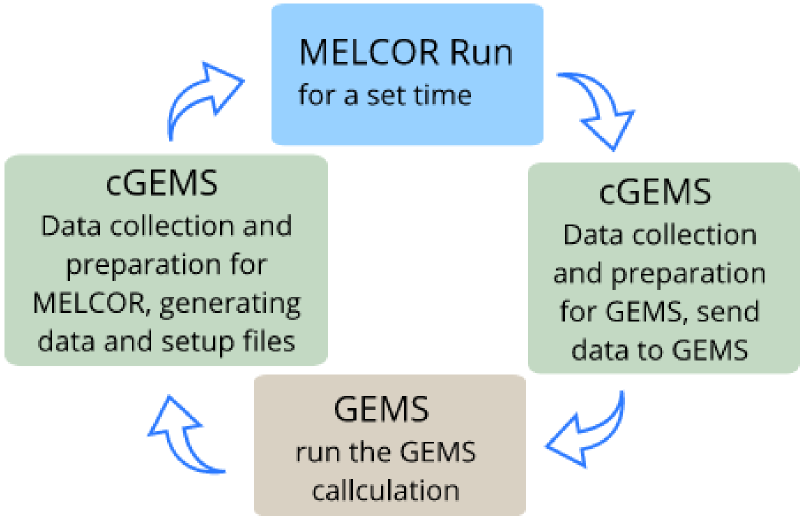
Alexis de Villepin, Internship Report, PSI, 2024

Couple GEMS with MELCOR, cGEMS

Couple two systems

- Idea is to provide MELCOR with a better information about speciation and, for example, vapour pressures.
- Should provide more accurate chemical description and deepen our understanding of fission products behaviour and release





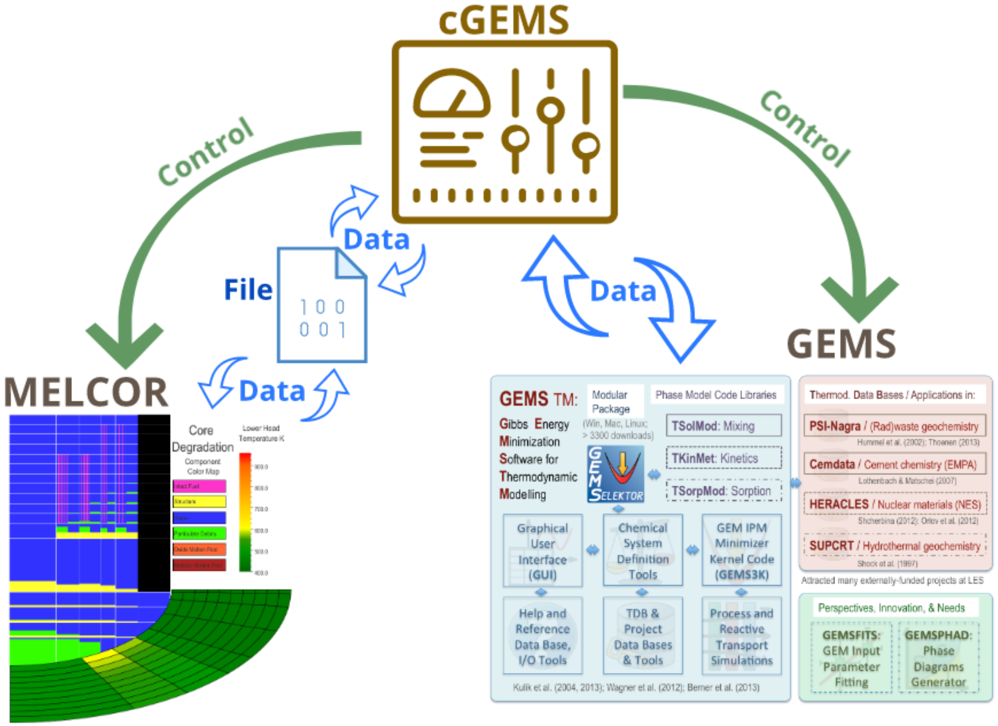
Simulation flow

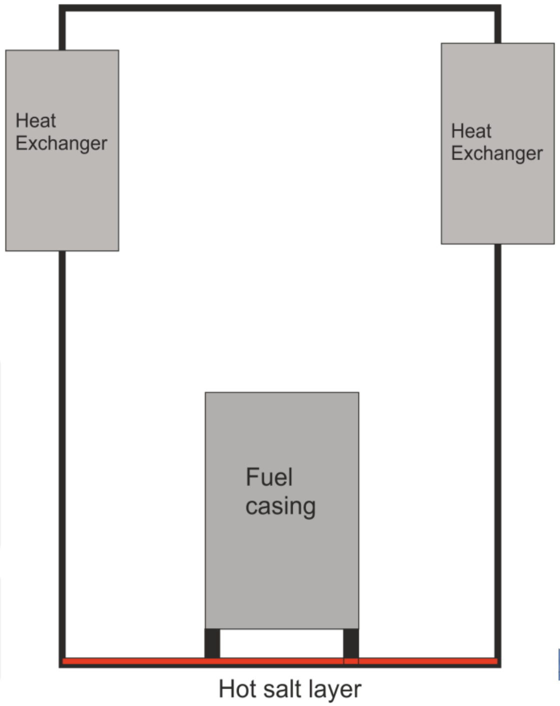
- The simulation “flow" is done in time steps. This means, after MELCOR was running for some time it stops, passes information to GEMS, GEMS does the TD modelling and passes the information to MELCOR. Repeat.

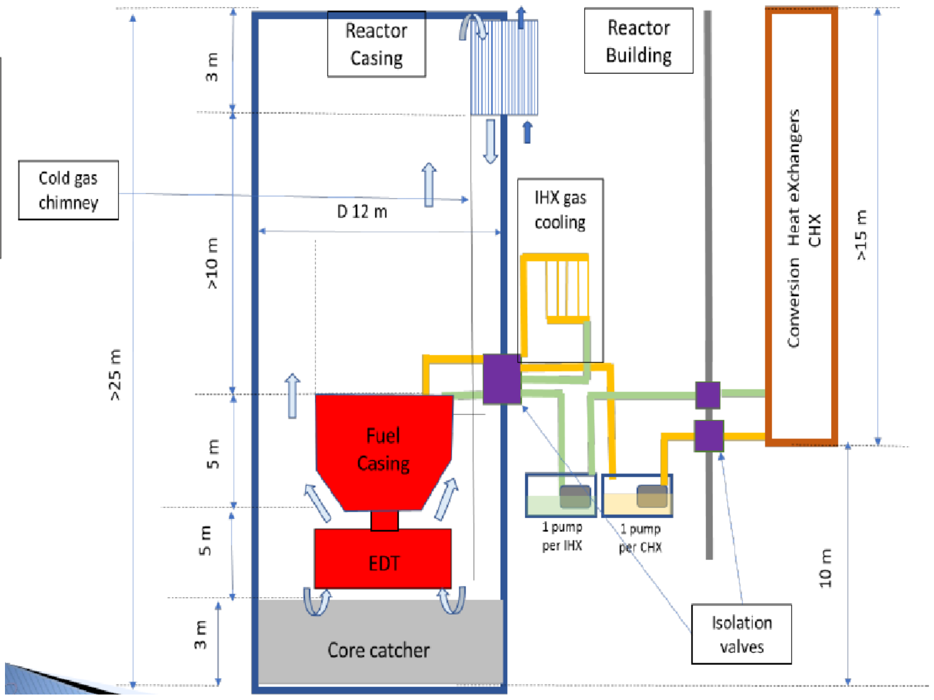
cGEMS application to severe accident in MSFR

Within EU project SAMOSAFER the deliverable: **Aerosols formation and filtration in accidental conditions** was resealed. It is not public, but the results have been also in Journal of Nuclear Materials:
J. Kalilainen, S. Nichenko, J. Krepel:
“Evaporation of materials from the molten salt reactor fuel under elevated temperatures”
https://doi.org/10.1016/j.jnucmat.2020.152134

Simple salt spilling scenario in cylindrical containment with salt heat up from 800°C to 1500°C.





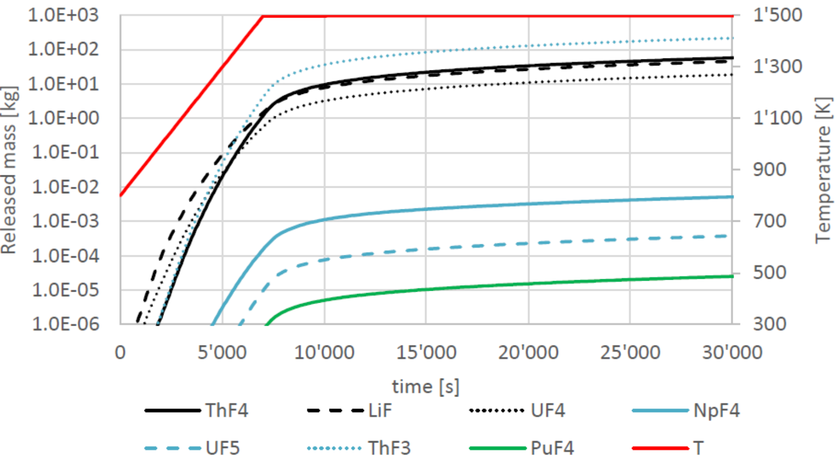


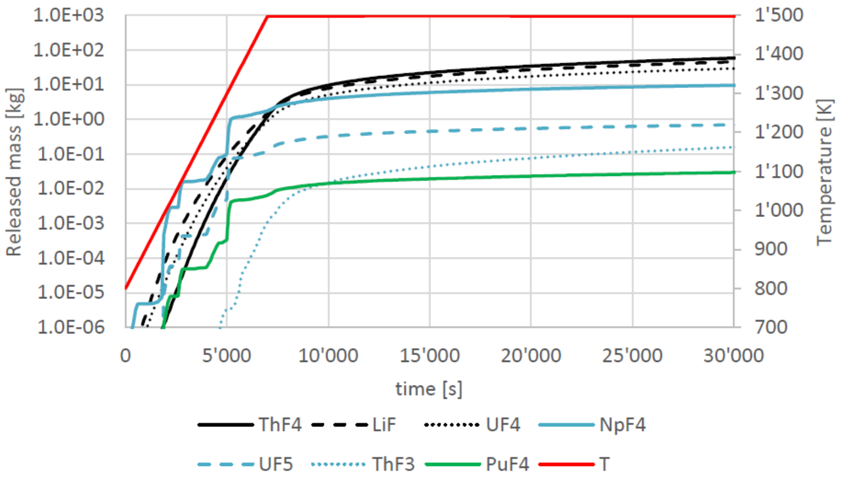
From the SAMOFAR Final meeting, E. Merle et al.

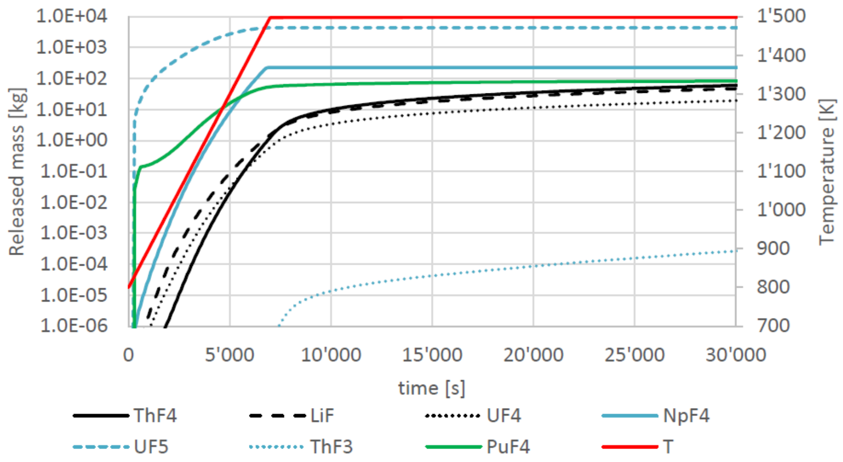
Released mass sensitivity to redox

ETH zürich PSI

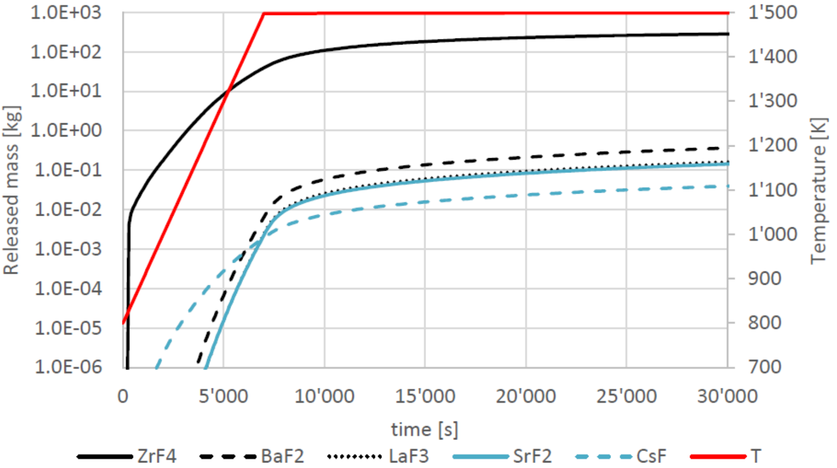
Fluorine: -1% mol. | Stoichiometric | +1% mol.

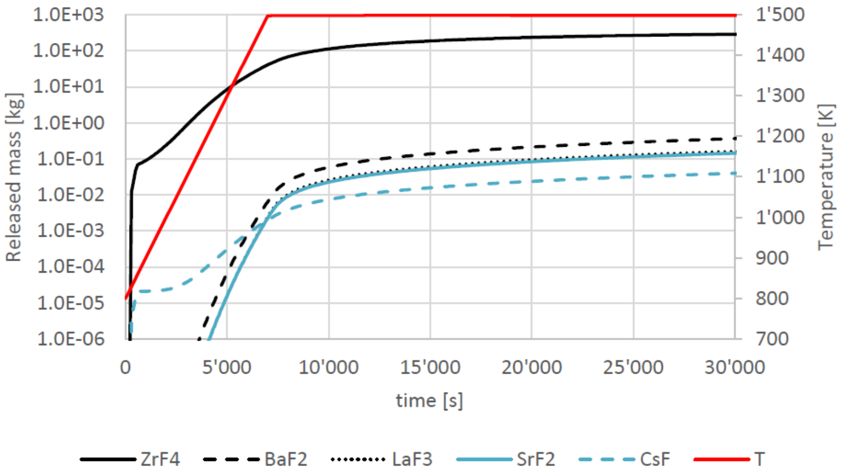


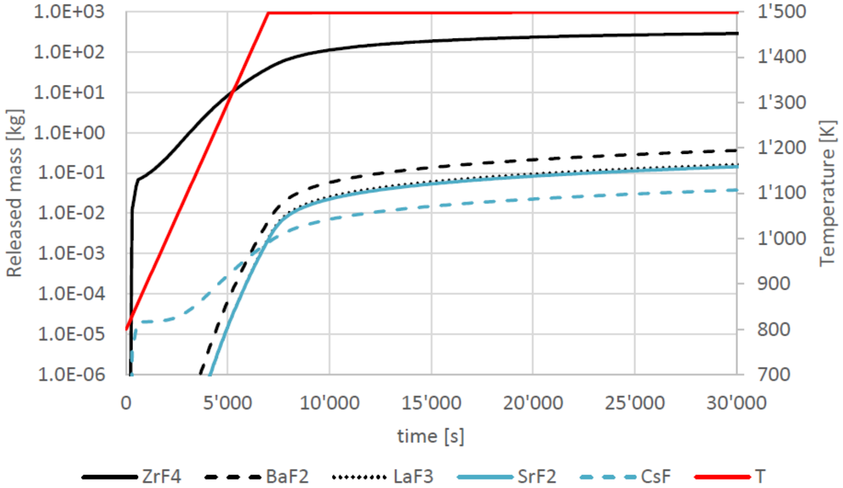




Actinides and salt species







Fission products species

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

5 major fissile materials to start the Th-U cycle

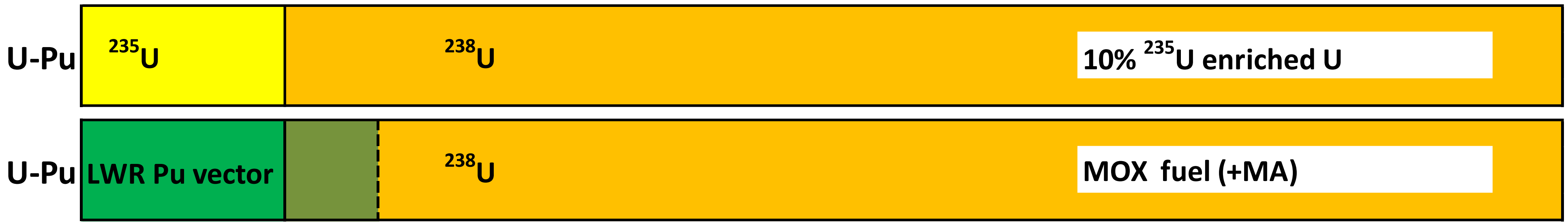
Material	RG_Pu	LEU	HEU	U233	WG_Pu
Fissile isotope(s)	^{239}Pu, ^{241}Pu	^{235}U	^{235}U	^{233}U	^{239}Pu
Fissile isotope share	~60%	1-20%	21-95%	60-100%	>93%
"Availability"	medium	high	high	low	medium
Proliferation risk	medium	medium	high	high	high

RG_Pu and LEU as initial fuel load

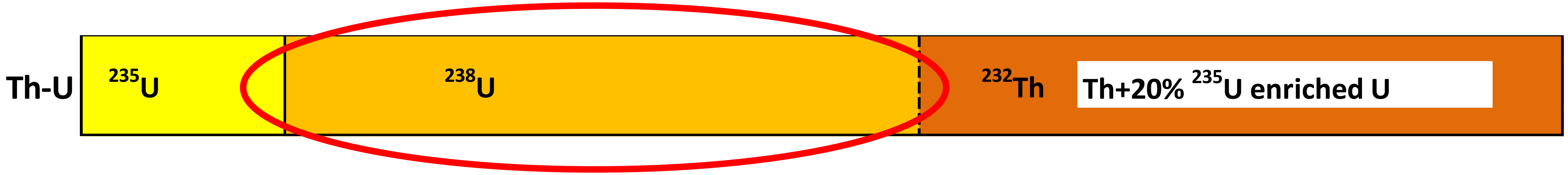
PSI

- Both **RG_Pu** and **LEU** are very natural option to start the **U-Pu** cycle.

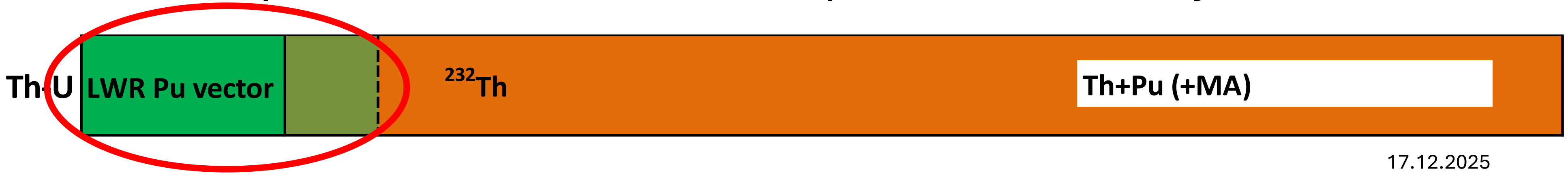
Fuel composition - initial cycles (10% ^{235}U equivalent)



- Starting **Th-U** cycle with **LEU** induces **^{238}U presence** in the core.

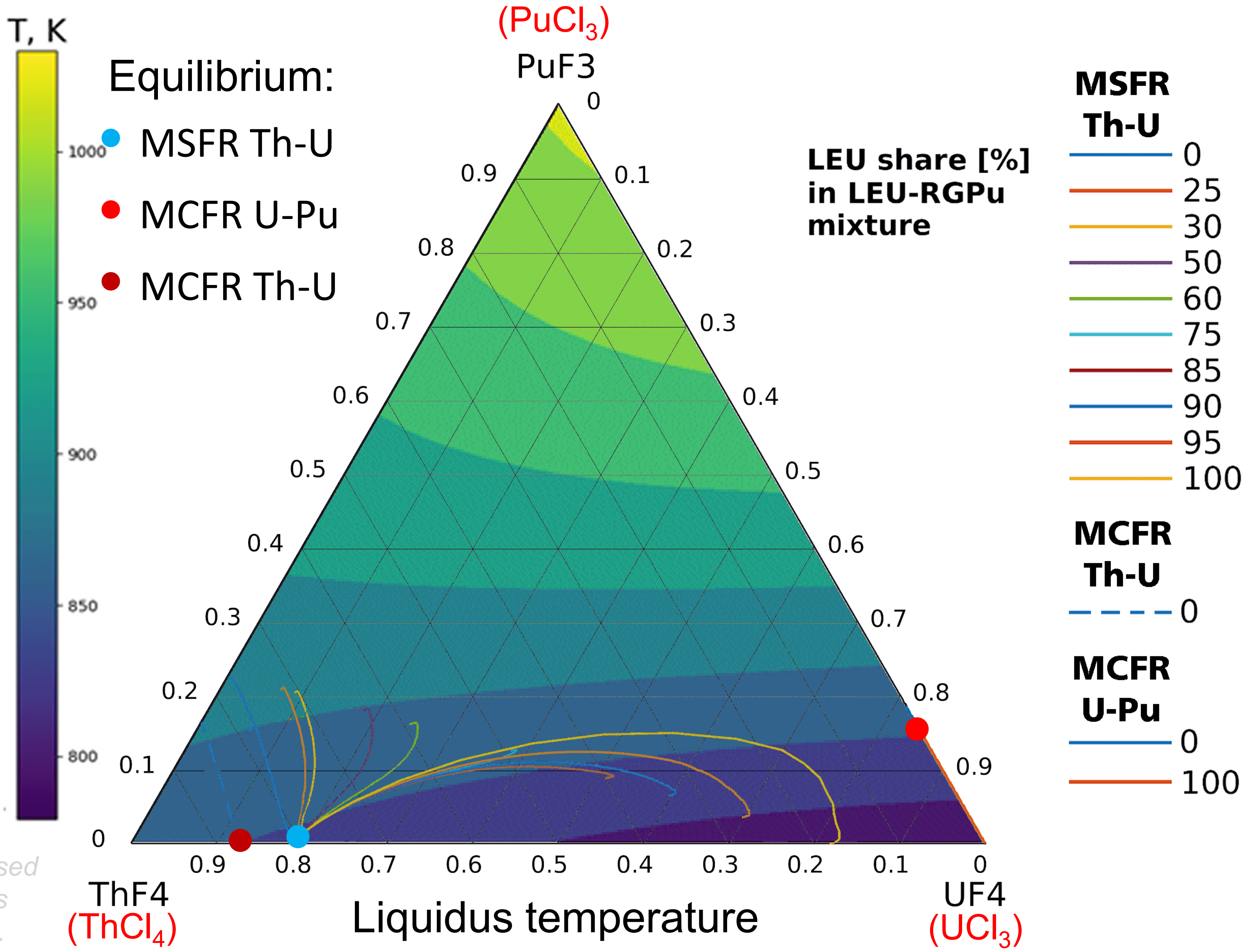


- Starting **Th-U** cycle with **RG_Pu, LEU** or their mixture introduces strong **perturbation.**
- **Pu and $^{235\ \&\ 238}U$** are not presented in the salt at equilibrium Th-U cycle.



Transition to Th-U cycle in MSFR (and U-Pu MCFR)

PSI

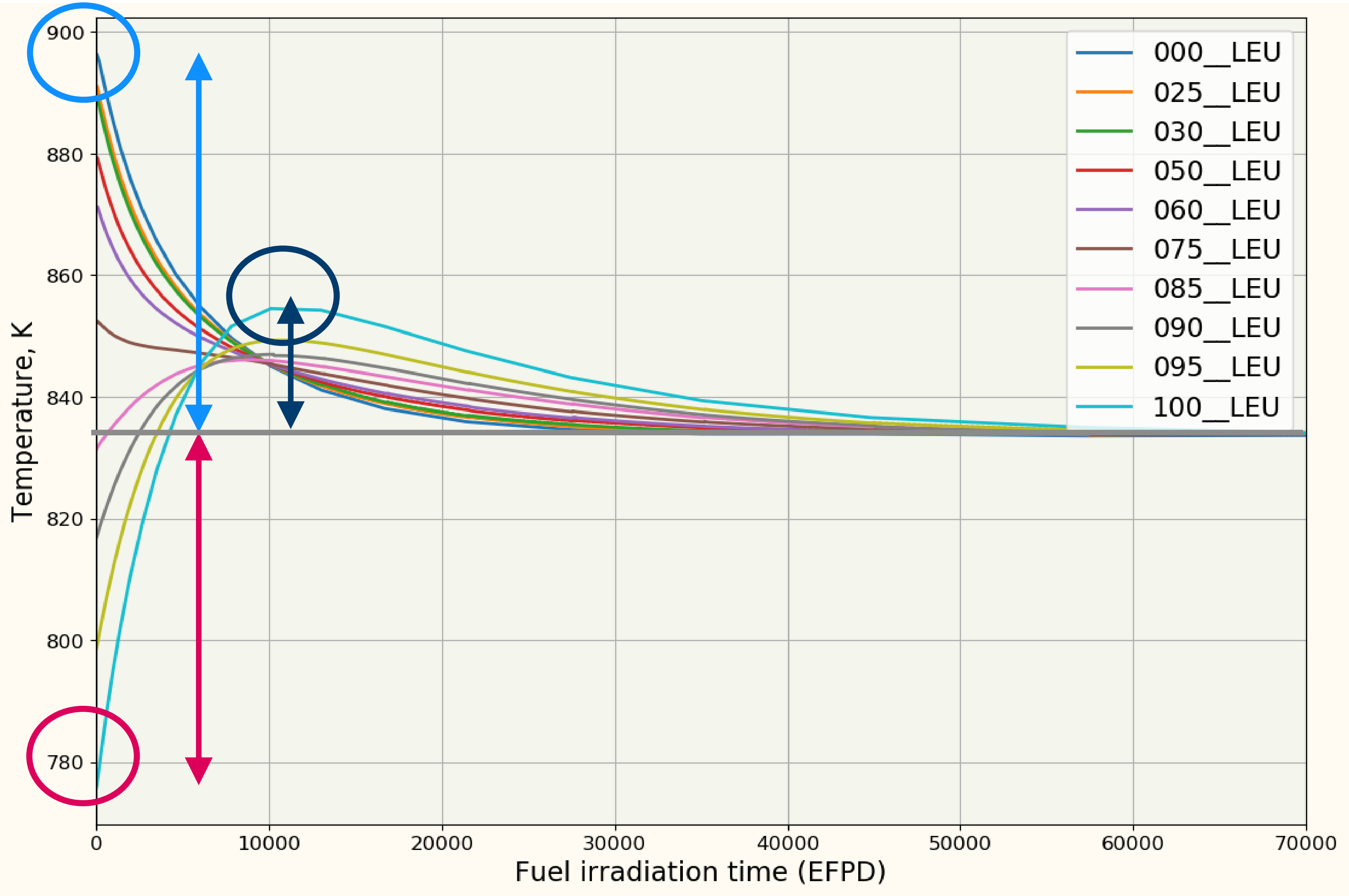


Křepel, J. et al., Transition to closed Th-U fuel cycle in fluoride salts based fast MSR. ICAPP 2019.

Evolution of the liquidus temperature

- **PuF_3** presence increases the liquidus temperature.
- **UF_4** presence decreases the liquidus temperature.
- The temperature for equilibrium Th-U cycle is cca **835K.**
- The difference is:
  up to **-55K** and **+60K** or **+20K**.

LiF-ThF4-UF4-PuF3 (at **76.6%** LiF).



Křepel, J. et al., Transition to closed Th-U fuel cycle in fluoride salts based fast MSR. ICAPP 2019.

PSI Center for Scientific Computing, Theory and Data

Thank you

Jiri Krepel, Sergii Nichenko, Mateusz Malicki, Alexis de Villepin
21 July – 25 July 2025, IAEA, Vienna