PAUL SCHERRER INSTITUT

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MSR fuel cycle and thermo-dynamics simulations

International Conference on Fast Reactors and Related Fuel Cycles: Sustainable Clean Energy for the Future (FR22)

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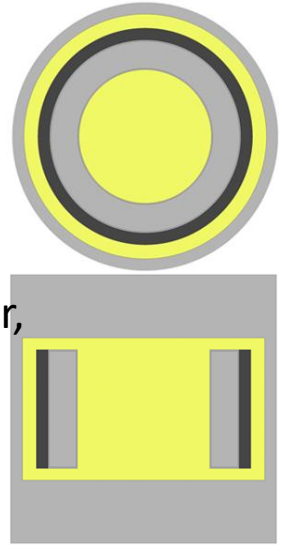
Introduction

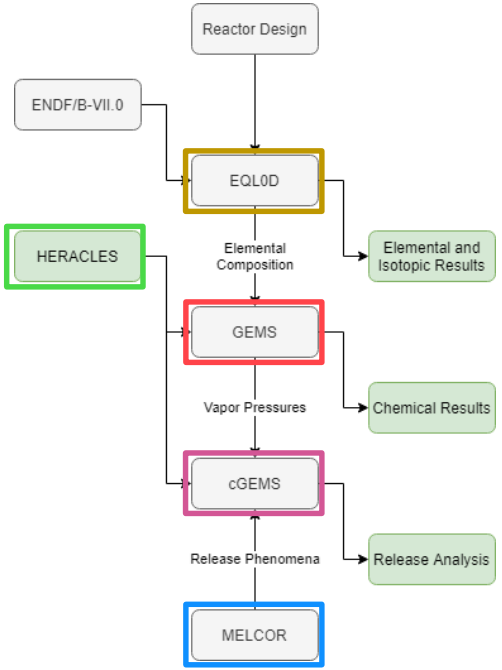
- **Molten Salt Reactors** with liquid fuel have potential to combine **excellent fuel cycle** capabilities with novel **safety performance**.
- However, many proposed concepts are based solely on **neutronic simulations** and salt **melting temperature** consideration.
- In this study, we tried to go little bit beyond this simple approach.
- MSR neutronic simulations were combined with thermo-dynamics calculations and with simplified severe accident simulation.
- Focusing on class of homogenous MSR, where both U-Pu and Th-U closed cycles were considered in both fluorides and chlorides salts.

Interconnection of applied tools

- Neutronic simulation: PSI in house procedure EQL0D.
- Thermo-dynamic calculation: PSI in house code GEMS.
- With updated Heracles database.
- Severe accident simulation: cGEMS code
  It is a loose coupling of GEMS
  and MELCOR code.
- Neutronic input data: MSFR-like geometry, replacement of blanket by Hastelloy reflector, 3GWth power, and EVOL benchmark reprocessing specification.

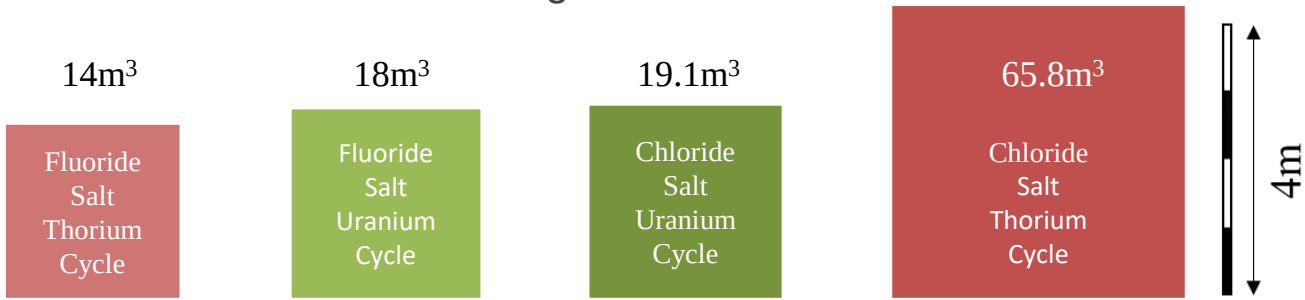


MSFR-like geometry



Neutronic simulation

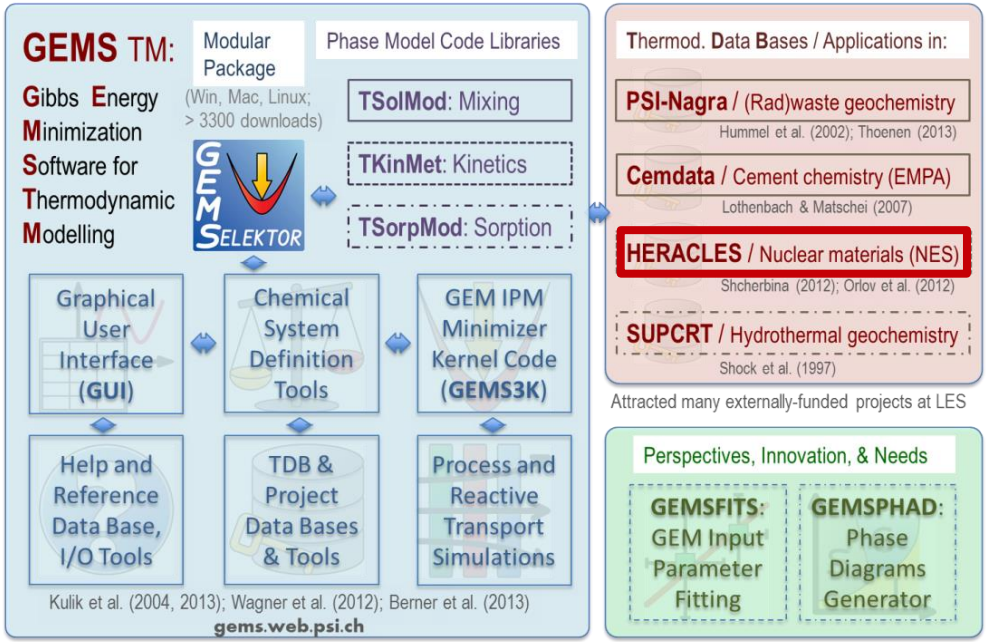
- Acknowledgement: it is continuation of B. Hombourger PhD thesis published in 2018.
- Minimal critical size of an iso-breeding reactor was estimated.
- As well as major components of the fuel salt:



$77.5LiF-22.5UF_4$	$77.5LiF-22.5UF_4$	$68NaCl-32UCl_3$	$50NaCl-50ThCl_4$
Fluorides/Thorium	Fluorides/Uranium	Chlorides/Thorium	Chlorides/Uranium
F: 5.15E-02	F: 4.87E-02	Cl: 2.21E-02	Cl: 2.15E-02
Li: 2.43E-02	Li: 2.01E-02	Na: 4.62E-03	Na: 8.88E-03
Th: 5.51E-03	U: 5.60E-03	Th: 3.77E-03	U: 3.46E-03
U: 1.05E-03	Pu: 1.59E-03	U: 4.60E-04	Pu: 6.74E-04
Pu: 2.64E-04	Am: 5.79E-05	Pu: 2.33E-04	Am: 1.74E-05
Zr: 3.90E-05	Cm: 2.88E-05	Am: 3.94E-05	Zr: 1.57E-05
Am: 3.14E-05	Zr: 1.76E-05	Np: 1.08E-05	Nd: 1.24E-05
Cm: 2.53E-05	Nd: 1.43E-05	Zr: 7.28E-06	Cm: 1.05E-05
Nd: 2.07E-05	Ce: 1.12E-05	Cm: 6.63E-06	Ce: 9.66E-06
Ce: 1.88E-05	Np: 6.65E-06	Nd: 4.29E-06	Pr: 3.99E-06
Pa: 1.30E-05	Pr: 4.56E-06	Ce: 3.86E-06	Np: 3.57E-06

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 modification.
- 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 Heracles updates

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

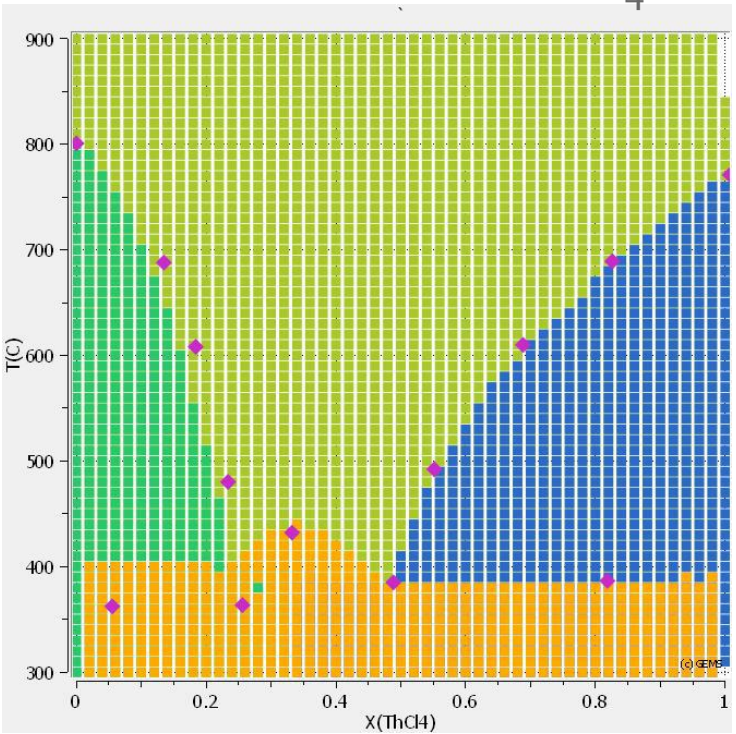
Additional Changes were made to: NpF_4, NdF_3, SrF_2, LaF_3, CeF_3, BaF_2, CsF

DIETZ, J., Chemical-Thermodynamic Modelling of the MSR-Related Systems Under Normal and Accident Conditions, MSc thesis, ETH Zurich, Switzerland, 2020

Extension of Heracles database for GEMS

1. Simulation based on parameters from literature (ideal mixing).
2. Tuning the first Redlich-Kister parameter.
3. Tuning the second Redlich-Kister parameter & formation enthalpies of intermediate compounds.
4. Optimization of excess Gibbs' energy curve.
5. Fine tuning.

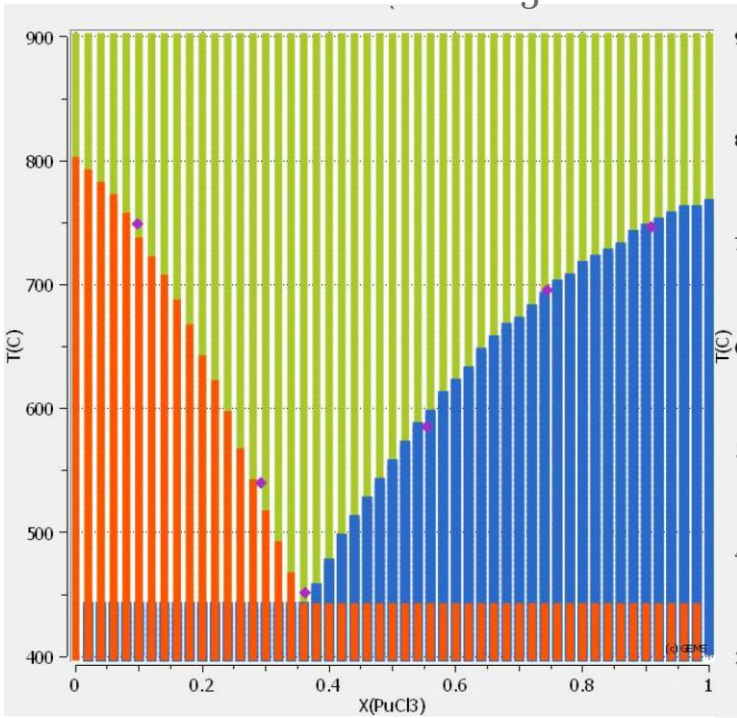
$NaCl\text{-}ThCl_4$



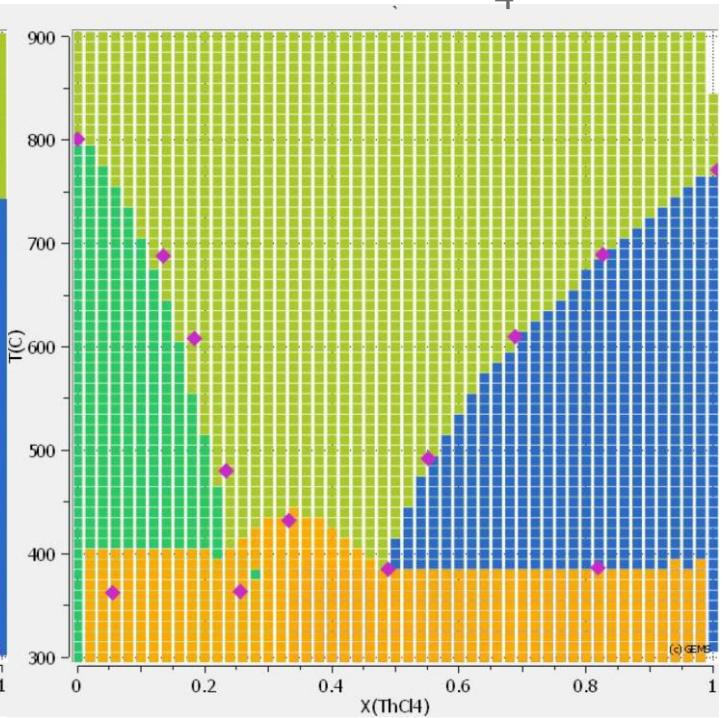
Extension of Heracles database for GEMS

- The aim was to cover two major reference salts:
- LiF-ThF_4-UF_4-PuF_3 for Fluorides and
- NaCl-$ThCl_4$-UCl_3-$PuCl_3$ for chlorides

$NaCl-PuCl_3$

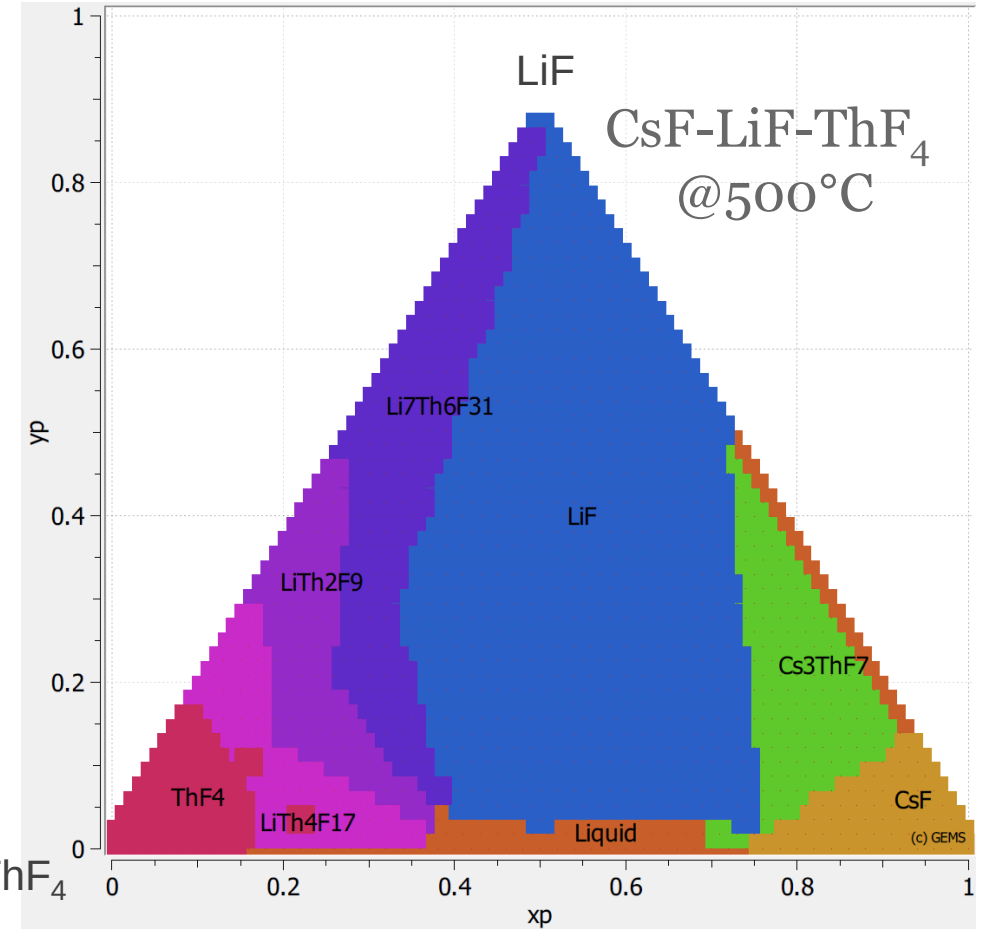


$NaCl-ThCl_4$



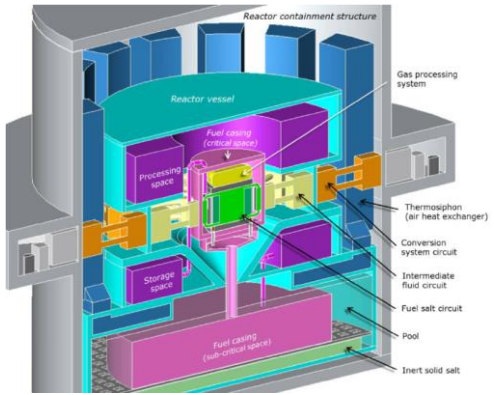
Extension of Heracles database for GEMS

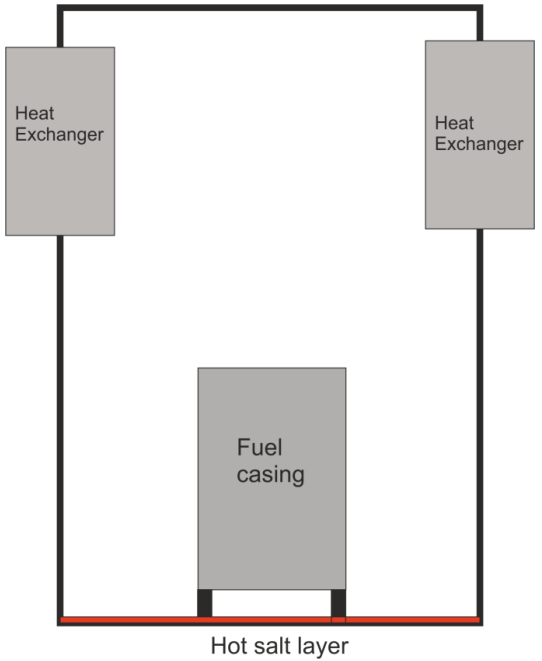
- The GEMS code phase-diagram plotting capability is still under development.
- Included is an example for the $CsF\text{-}LiF\text{-}ThF_4$ system at 500°C



Simulation of severe accident in MSFR

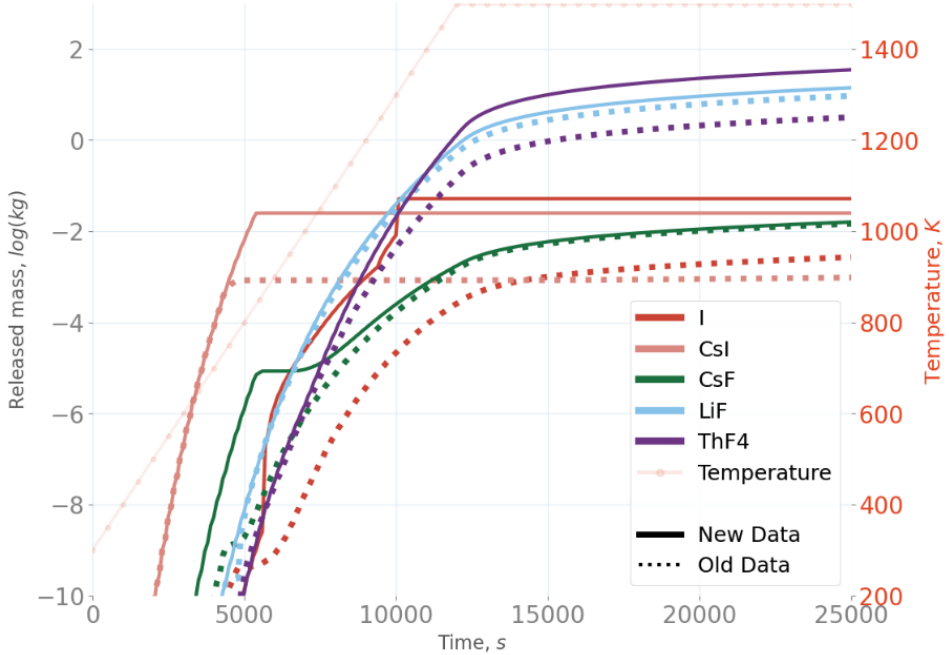
- Simplified assumption: salt complete spill to bottom of cylindrical containment and its heat up to 1500K in several hours.
- First results on the SAMOSAFER task 3.4 published in Journal of Nuclear Materials
  - J. Kalilainen, S. Nichenko, J. Krepel: "Evaporation of materials from the molten salt reactor fuel under elevated temperatures".





Result with updated Heracles database

- Cumulative release of various substances as a function of time was recalculated with the updated Heracles database.



Summary

- The major aim of this MSc thesis was a simulation of MSFR and MCFR like reactors operated in closed Th-U and U-Pu cycle.
- The minimal iso-breeder core size was estimated.
- The major compounds of equilibrium fuel composition were identified.
- The Heracles database of GEMS code was accordingly updated.
- GEMS code was used for several phase diagram simulations.
- cGEMS code was applied to simplified severe accident scenario with these updated data.

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Wir schaffen Wissen – heute für morgen

Thank you.

Questions?