JRCMSD – Thermodynamic database on Molten Salt Reactor systems

GTT Users' Meeting

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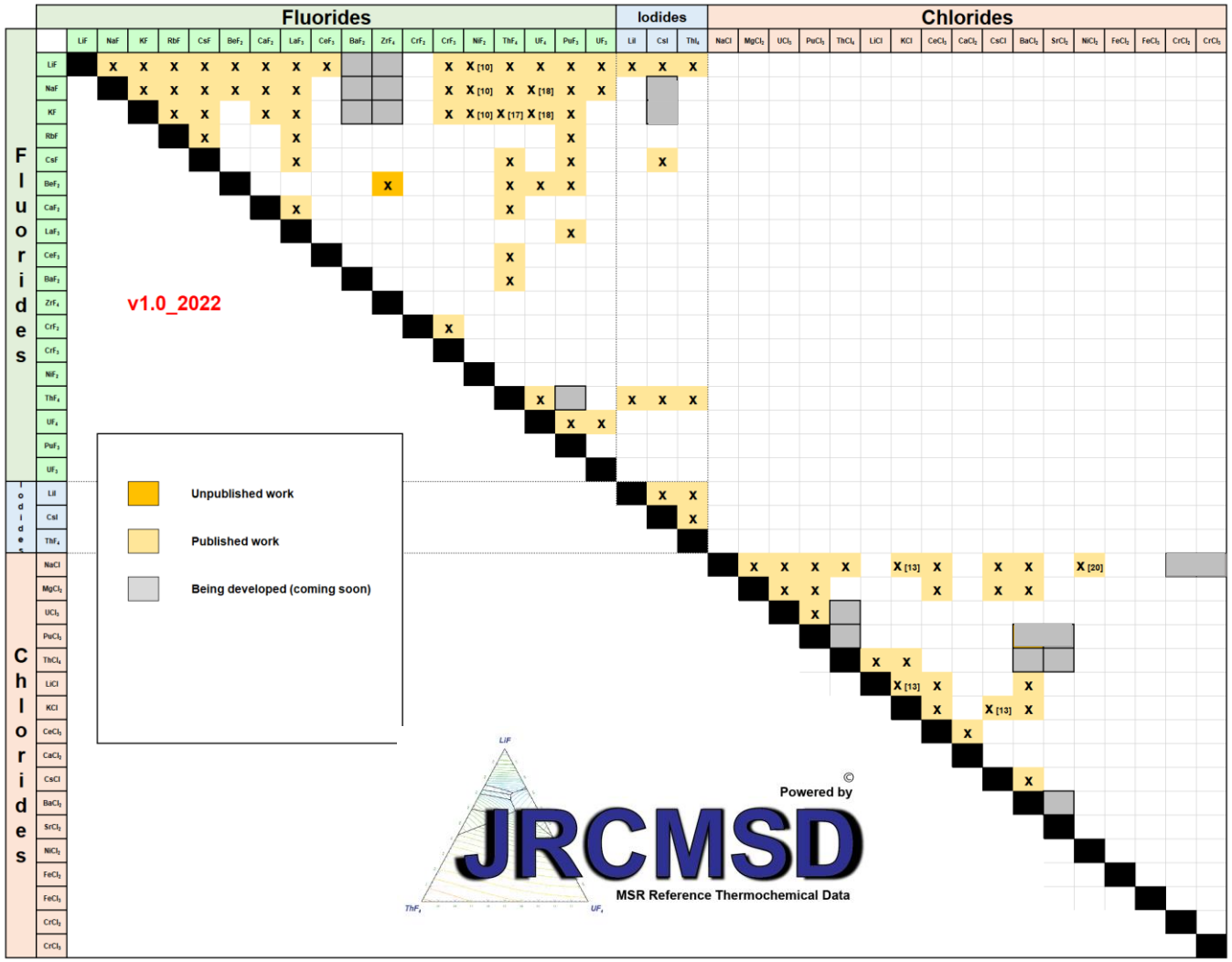
JRC Thermodynamic database - JRCMSD



- 108 binary systems included
- Describes main Molten Salt Reactor (MSR) Fuels and Coolants
- Covers Chlorides and Fluorides
- Multi-lateral collaboration TEMOSA Project
  - (CEA, JRC, Ontario Tech, Orano, TU Delft)
  - Open for other partners (CNL …)
- Constantly extended by novel experimental data
- Extended by fission and corrosion products

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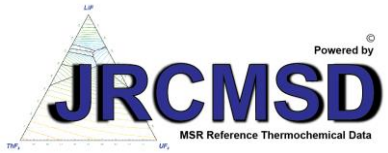
History of JRCMSD



- Started by JRC in 2002
- The idea was to describe the key fuel and coolant systems for MSR technology

- The liquid solution described by Pelton and Chartrand et al. quasi-chemical model based on quadruplet approximation
  - Model suitable for ionic liquids
  - Compatible with early developers

- In 2002-2018 developed mainly:
  - by JRC staff (*Benes, Konings*)
  - and PhD/Master students (*van der Meer, Benes, Beilmann, Capelli, Tosolin, Morelova, Schacherl ….*)

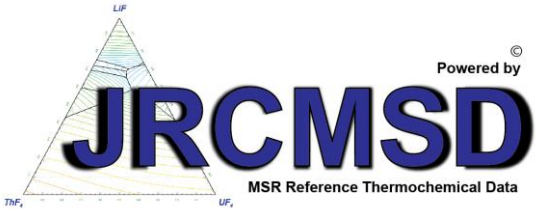
- ~2018 collaboration with TU Delft (*Smith*) started

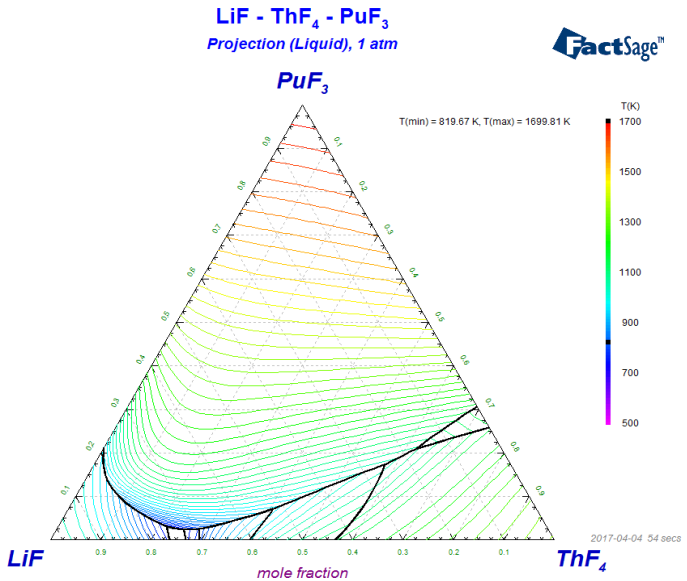
- 2022 TEMOSA project under preparation: multi lateral collaboration agreement to co-develop the JRCMSD including: *JRC, CEA, Ontario Tech., Orano group, TU Delft*

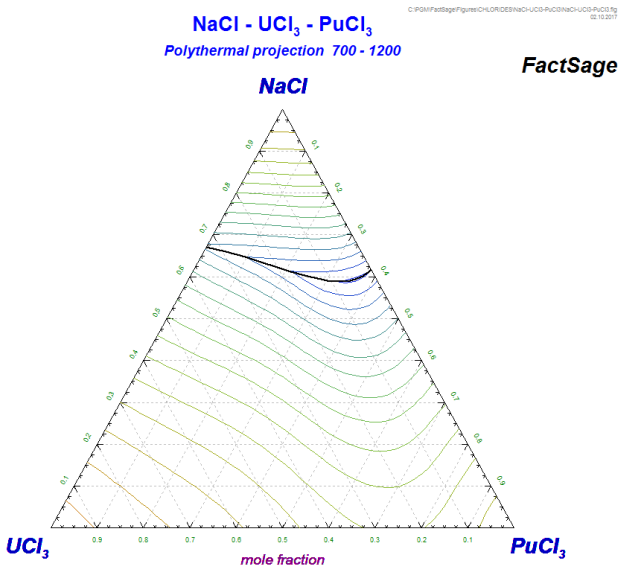
JRCMSD – Describes main MSR Fuel and Coolants

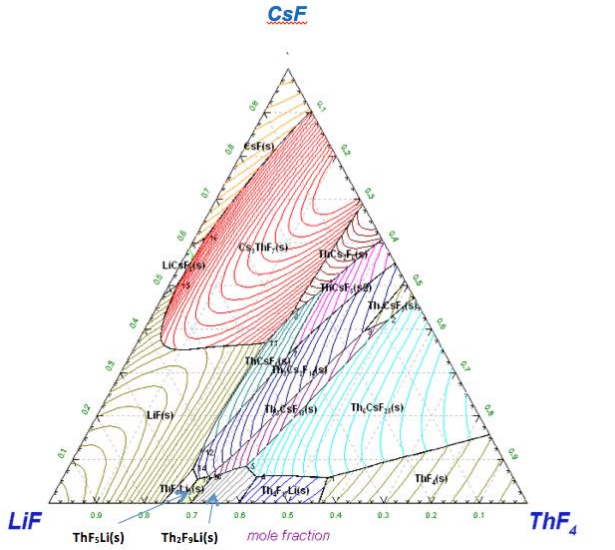
You can derive all Thermodynamic properties:

- Melting behaviour
- Heat capacity
- Vapour pressures
- Boiling boints
- Solubility of actinides and or corrosion/fission products
- Enthalpies of fusion (boiling, transitions)
- Mixing properties (how much heat you release or need to form the fuel mixture)
- **Great optimizing tool towards ideal Fuel composition**
- **… as well as to predict fuel behaviour during reactor operation (corrosion product + fission product influence)**









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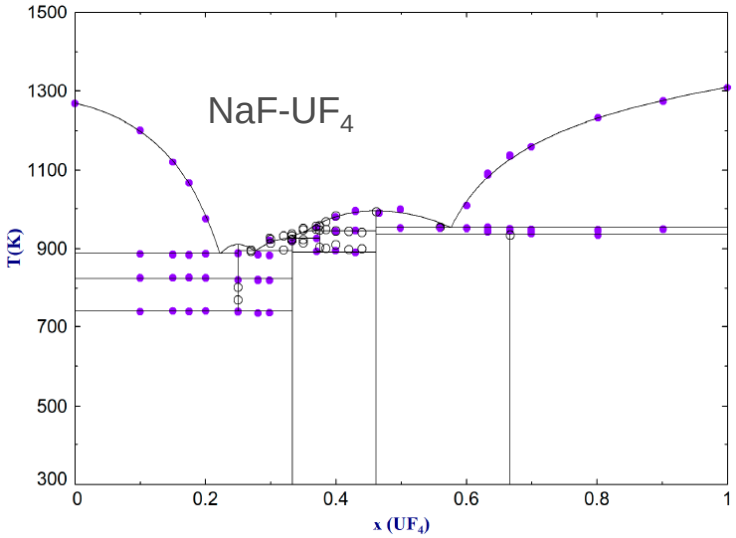
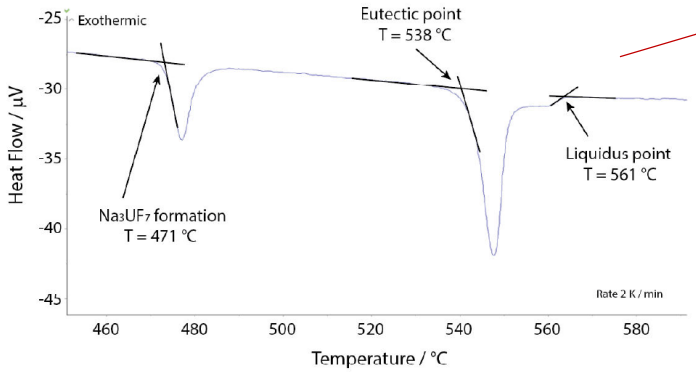
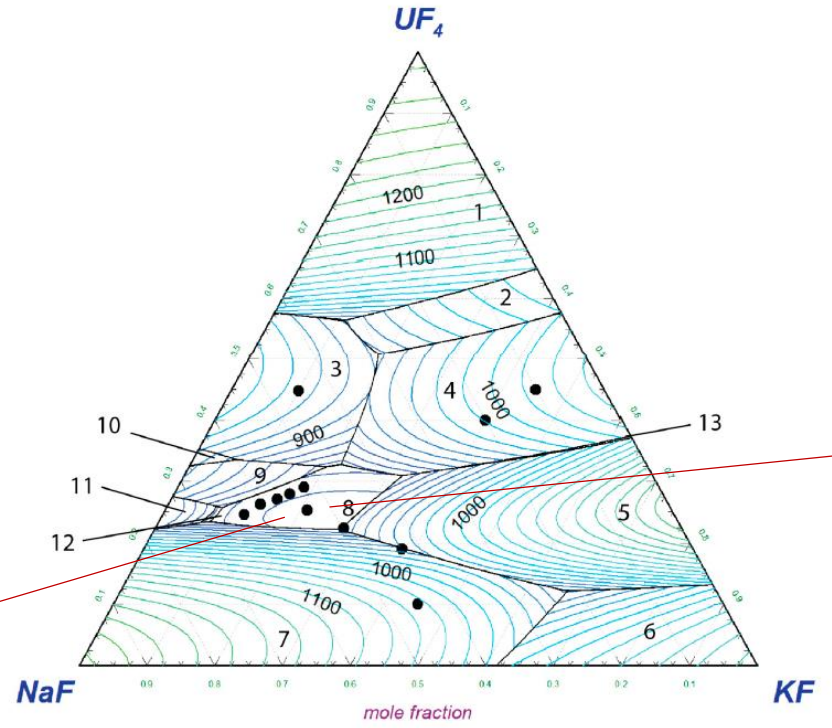
Example 1: Database Extension (Improvement)

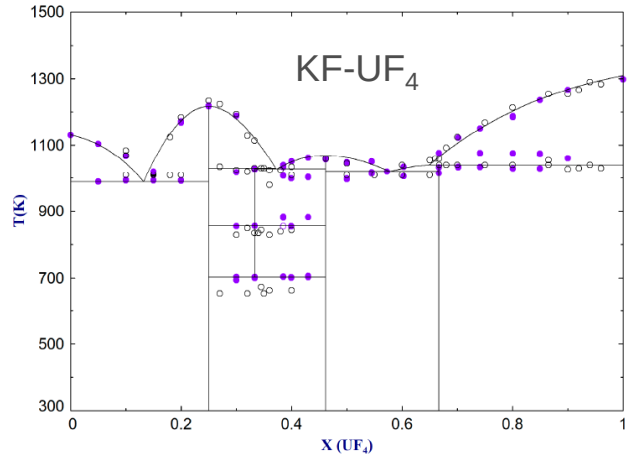
Re-assessment of the NaF-KF-UF_4 system

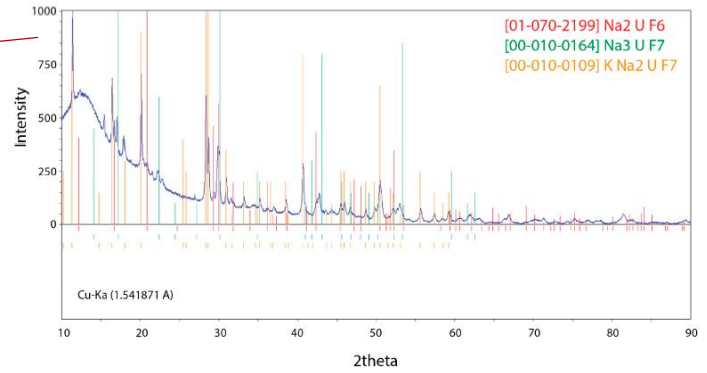
- Coupling own novel experimental data with Calphad optimization











XRD analysis of the NaF-KF-UF_4 (52.3-18.7-29.0 mol%) composition

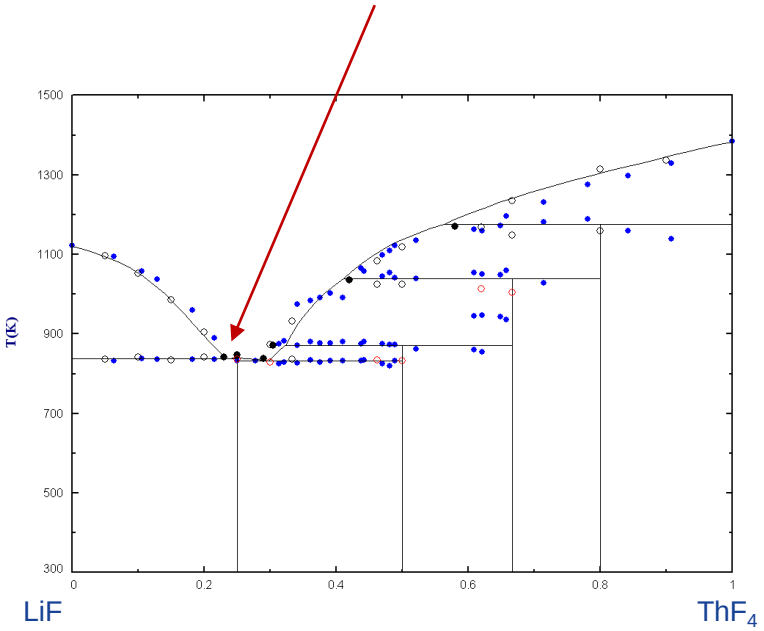
DSC measurement of the NaF-KF-UF_4 (52.3-18.7-29.0 mol%) composition

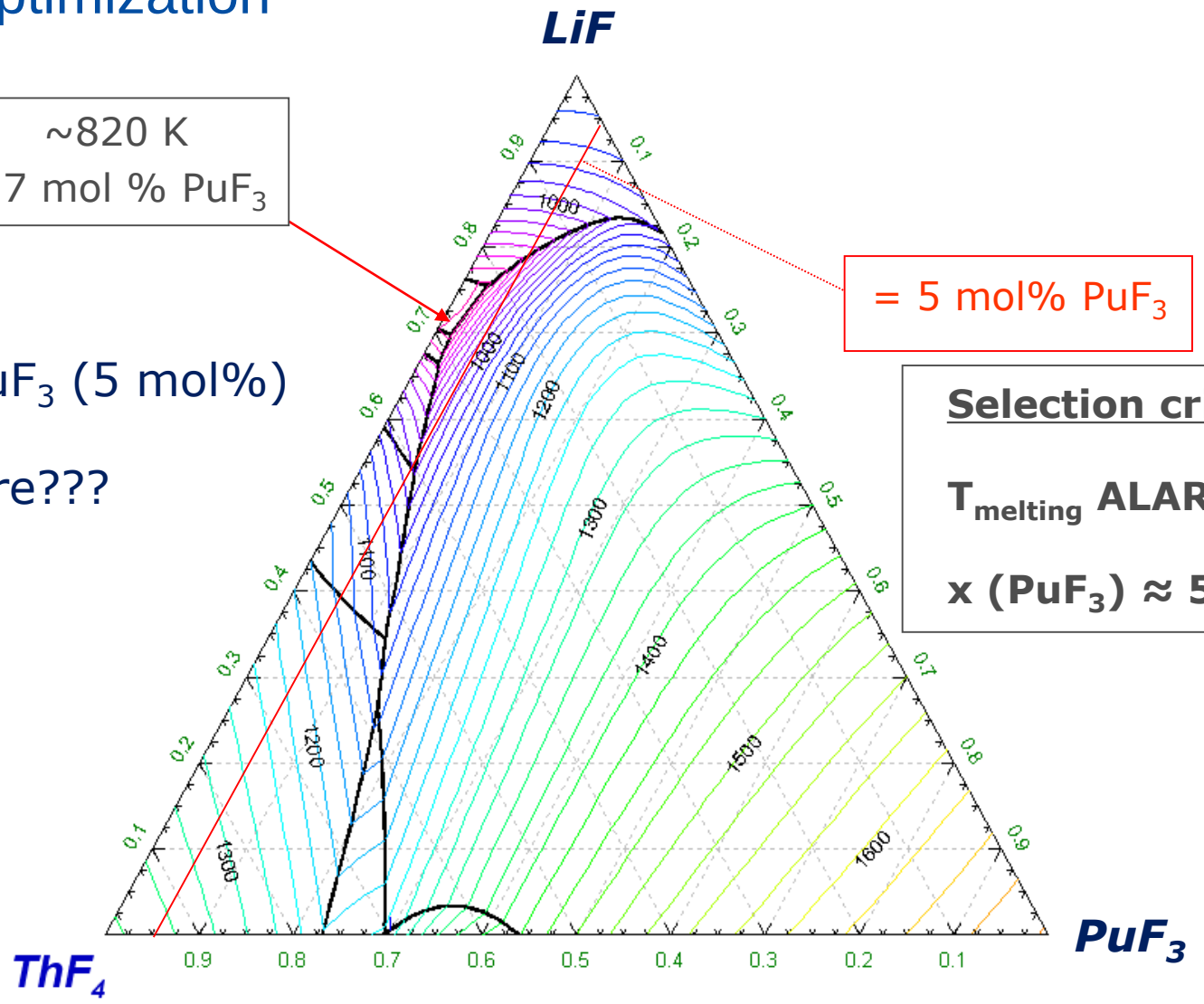
Example 2a: MSFR fuel optimization

~820 K
1.7 mol % PuF_3

= 5 mol% PuF_3

LiF-ThF_4 eutectic (78-22 mol%) + PuF_3 (5 mol%)
but ....
is this the lowest melting temperature???





Selection criteria:

$T_{melting}$ ALARA principle

x (PuF_3) ≈ 5 mol%

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Example 2b: MSFR fuel optimization

Reference system of the MSFR

$LiF\text{-}ThF_4\text{-}PuF_3$ (74-21-5 mol%) ... solvent is $LiF\text{-}ThF_4$ (78-22)

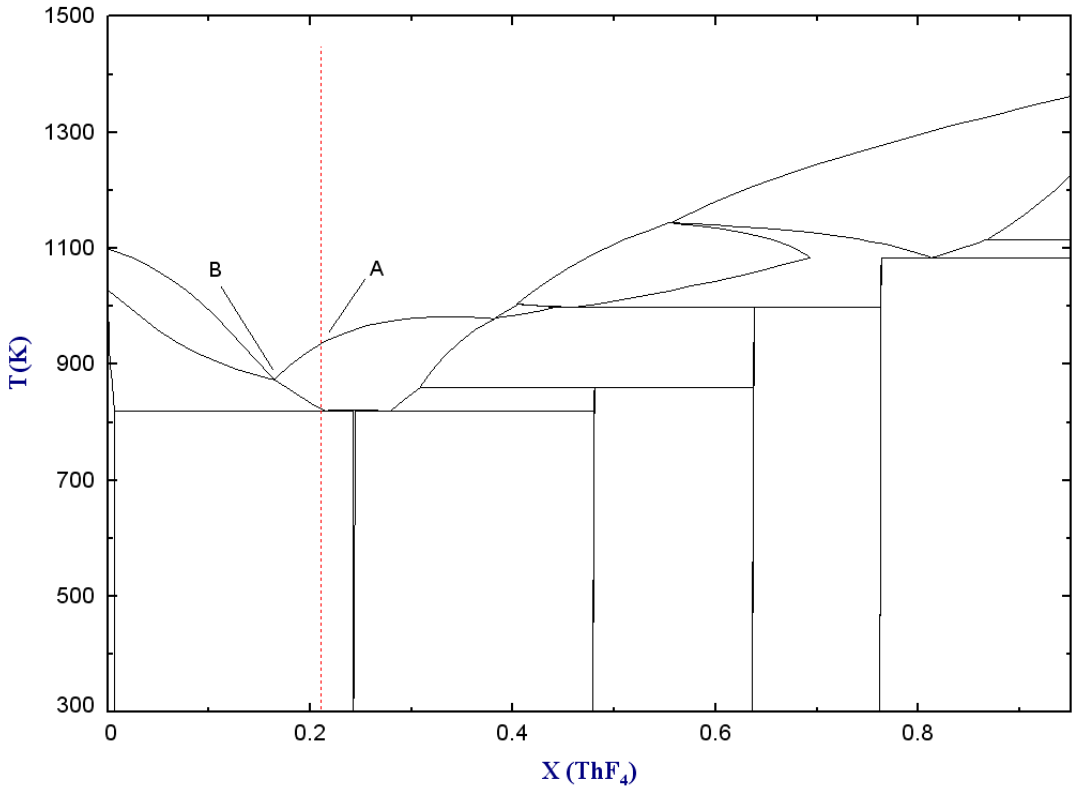
- liquidus point is **935 K** (662 ° C)
- inlet temperature is 985 K (712 ° C) (50K margin)

Point A

Point B

$LiF\text{-}ThF_4\text{-}PuF_3$ (78.6-16.4-5 mol%)

- liquidus point is **873 K** (600 ° C)
- inlet temperature is 923 K (650 ° C) (50K margin)



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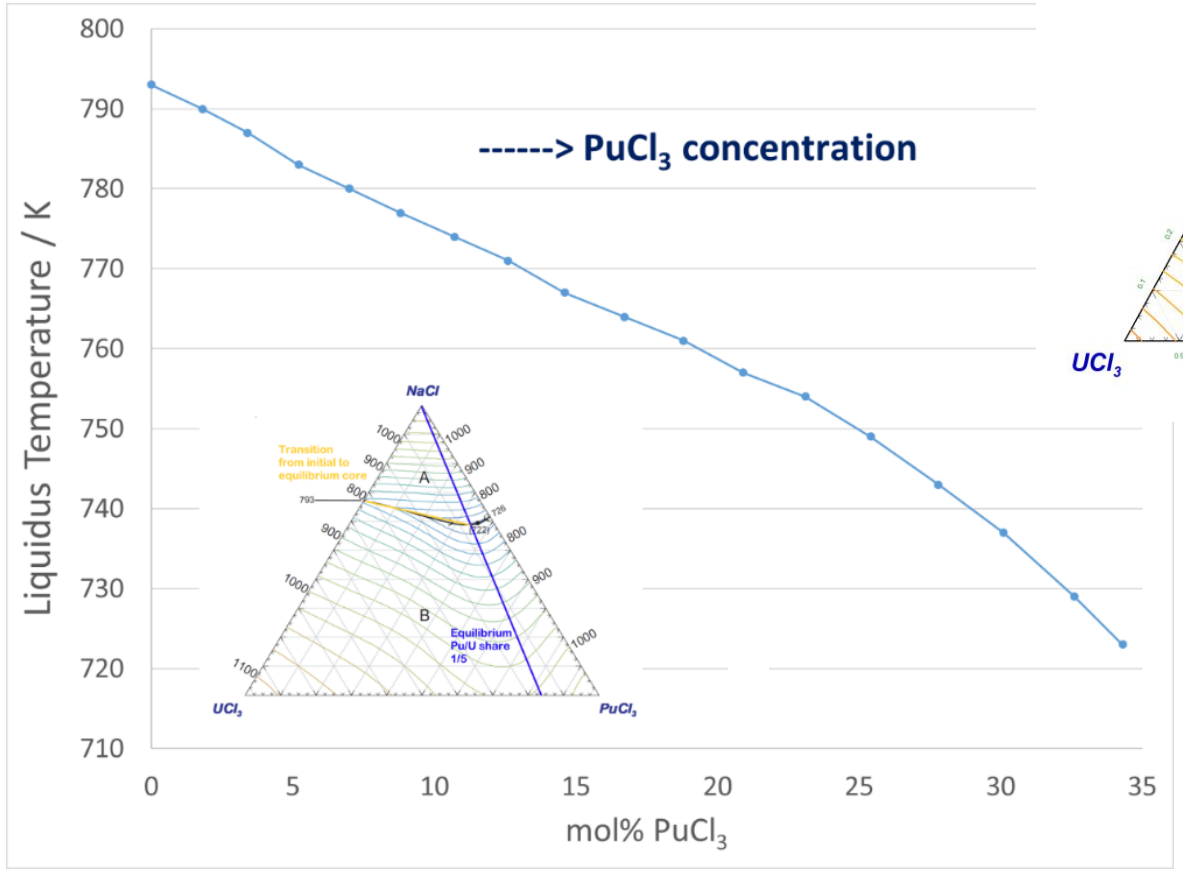
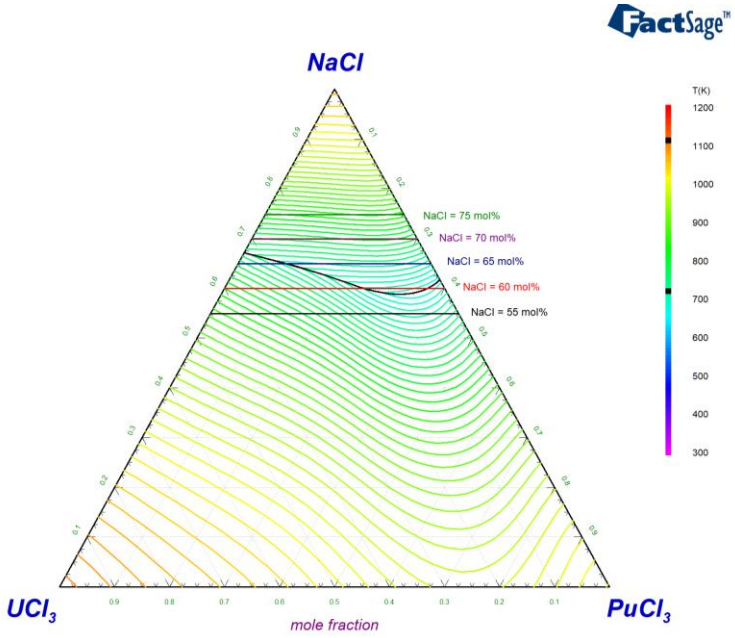
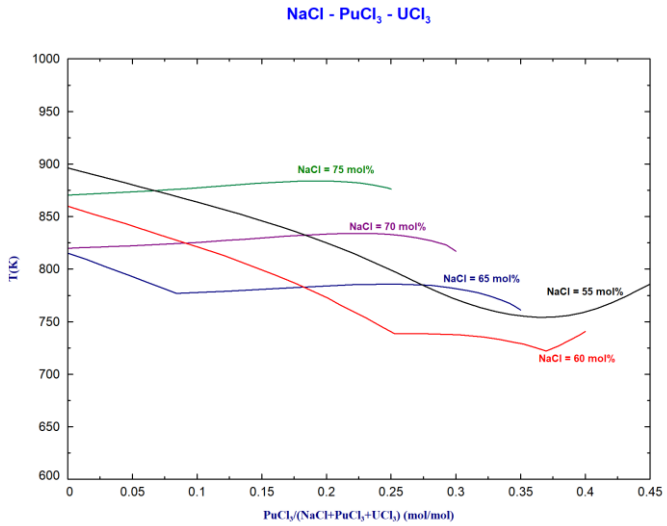
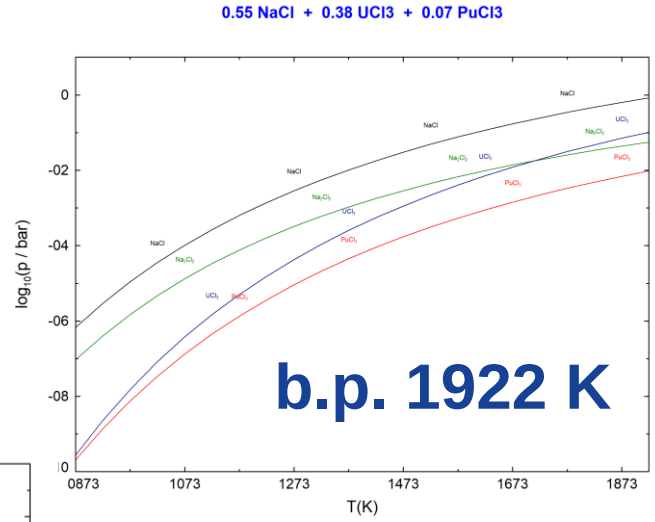
Example 3: Melting point and Vaporization behaviour

Frame: HORIZON2020 Project SAMOSAFER









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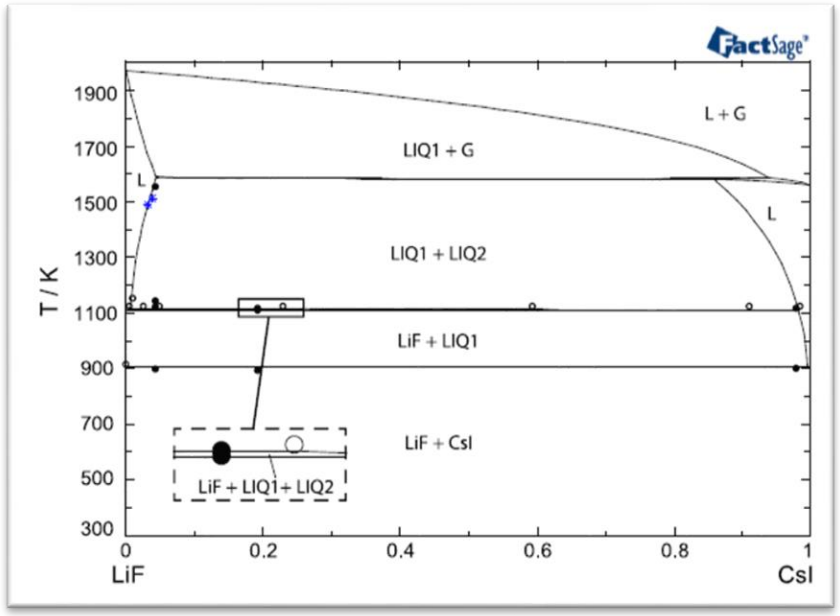
Example 4: Support to understand Cs and I release

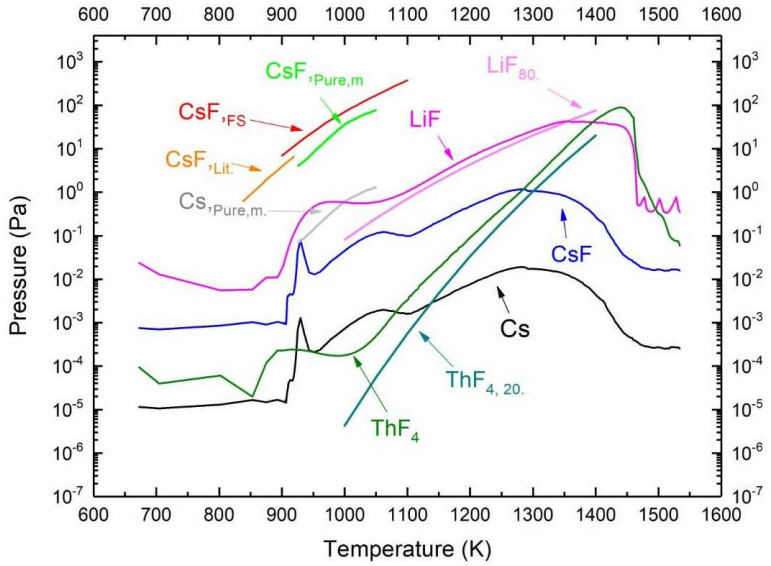
Fission Product retention of the MSR fuel

- 1 Determination of Fission product chemistry by simulation
- 2 Sim-fuel synthesis (CsI and CsF additives)
- 3 Measurement of CsF/CsI volatility using KEMS

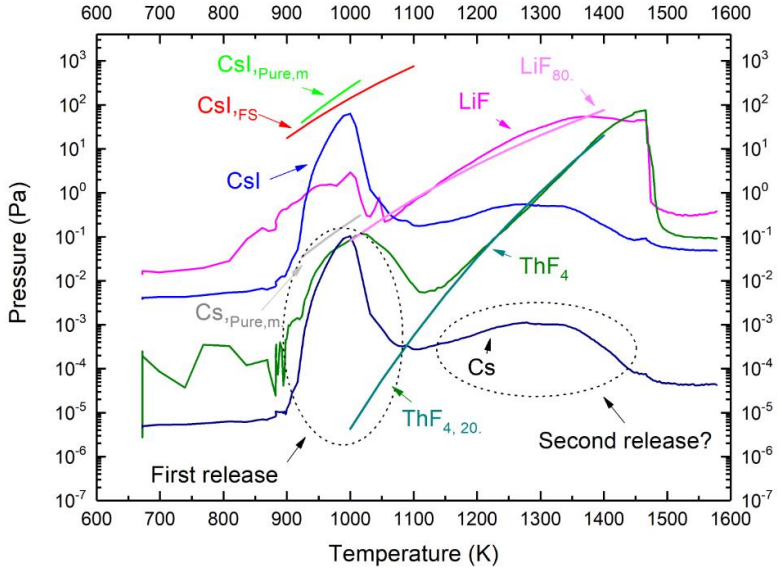
Frame: HORIZON2020 Project SAMOFAR (2015-2019)



CsF release from LiF-ThF4



CsI release from LiF-ThF4



Conclusions:

- CsF dissolves and as consequnce decreases volatility of Cs >100000x (ref. Elemental form)
- CsI is highly immiscible, but formation of CsI compound causes ~3000x lower volatility (ref. Elemental form)

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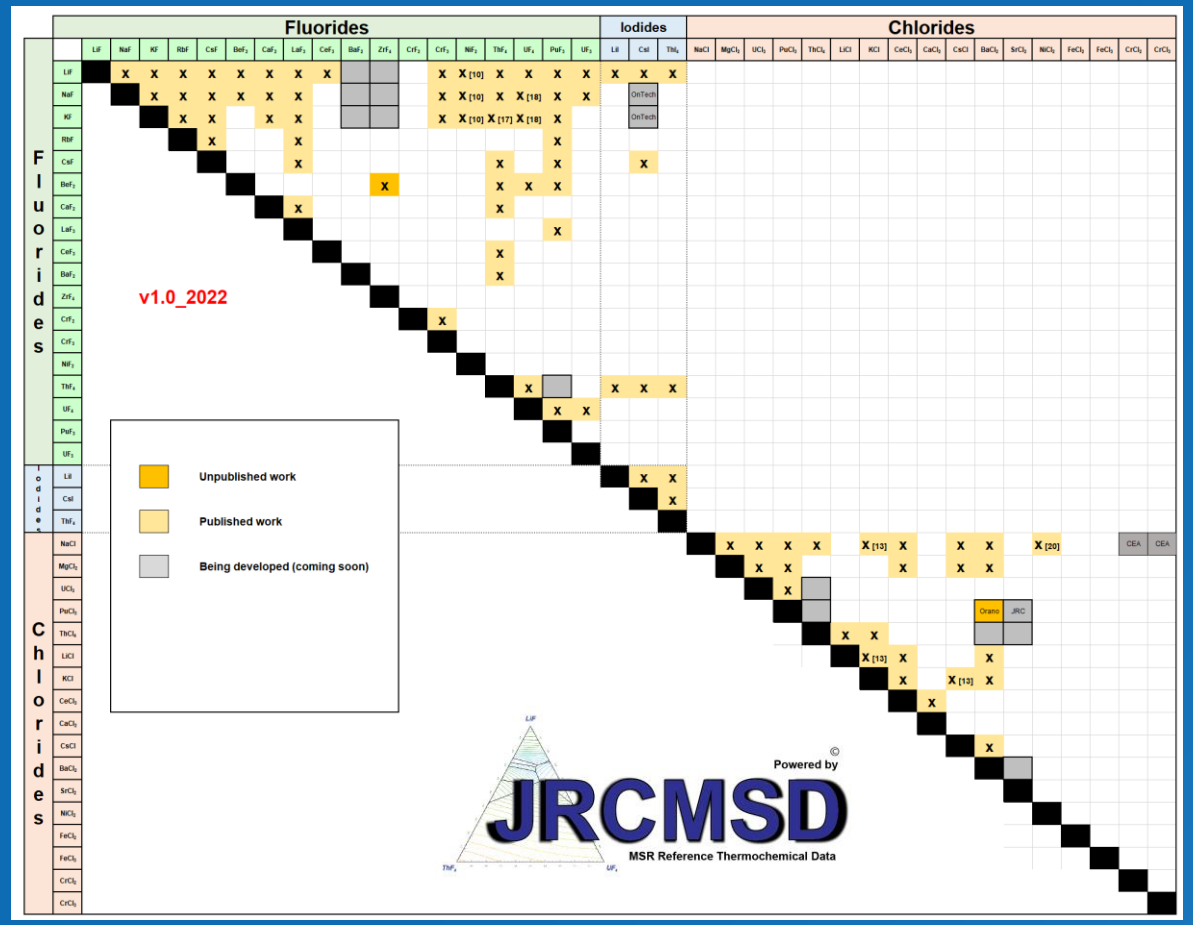
Summary



- Key MSR Fuel / Coolant salts covered
- Interaction with Fission and Corrosion products
- International development
- Open access via EU Science Hub (encryption by GTT)

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Thank you

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