



SAMOFAR Final Meeting

4 July 2019



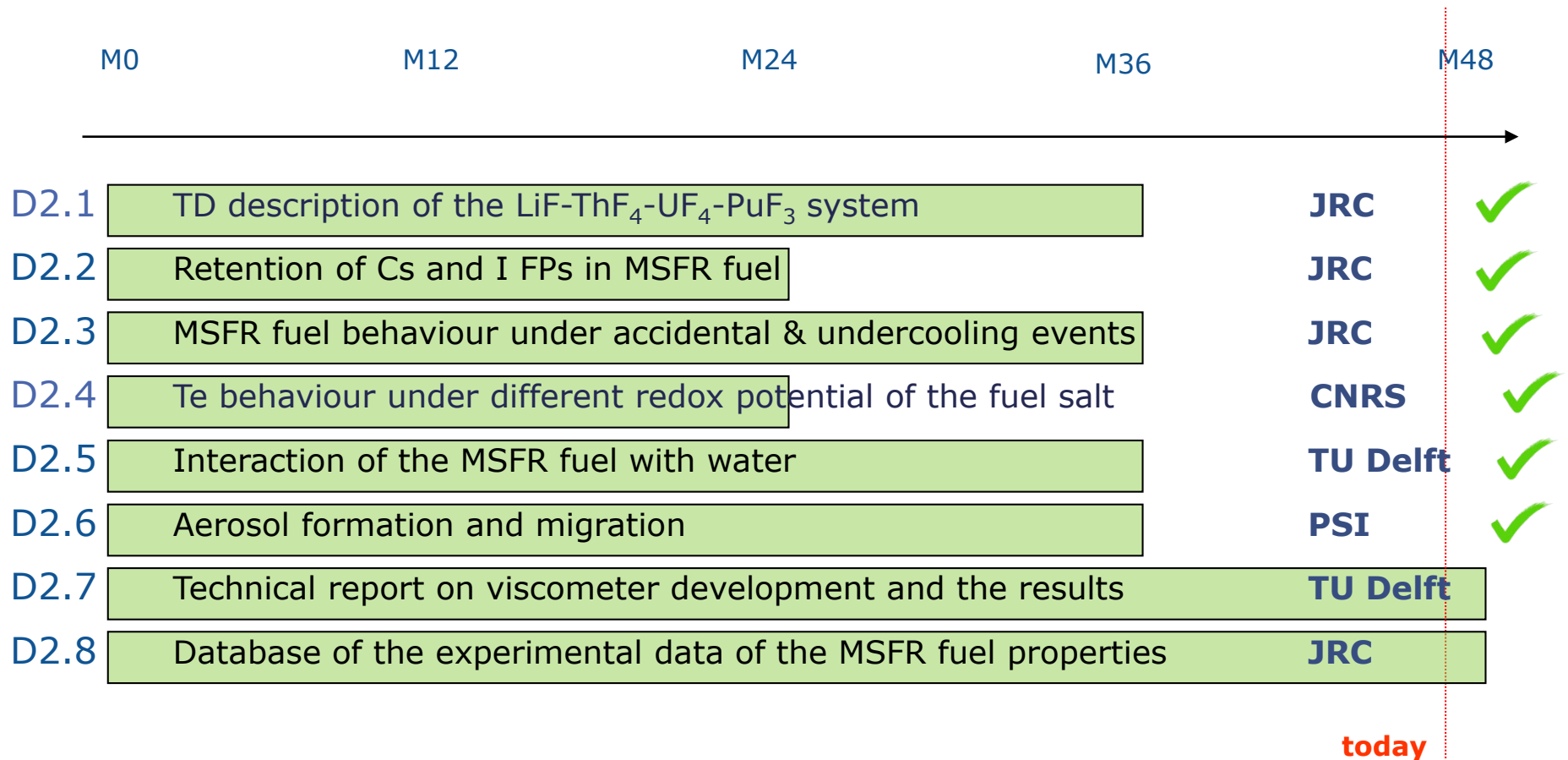
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WP2 Overview



Physical and chemical properties required for safety analysis

by Ondřej Beneš



Milestone 2.1

First experimental results with PuF_3 containing salt, verified by a publication of the results in a peer reviewed journal.

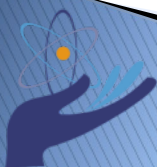
Responsible: JRC-ITU



Milestone 2.2

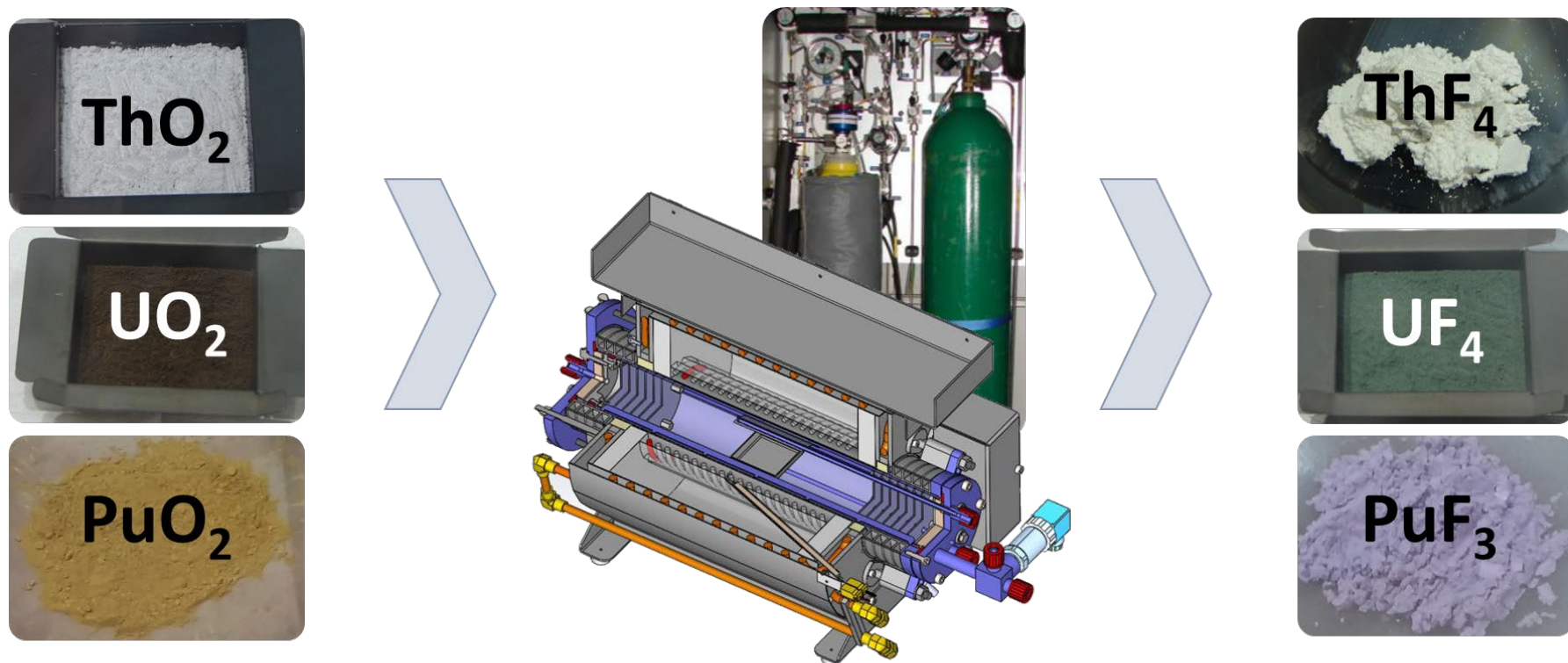
Viscometer prototype up and running, verified by first results on molten fluoride salts.

Responsible: TU Delft



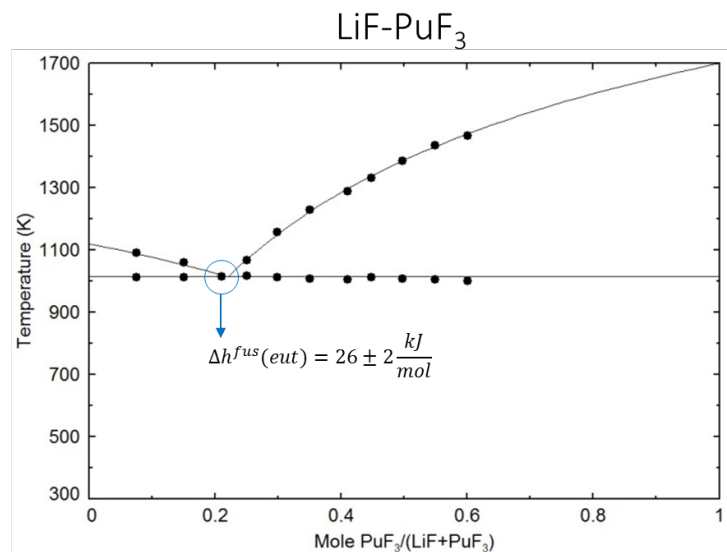
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Highlights: Actinide fluorides synthesis

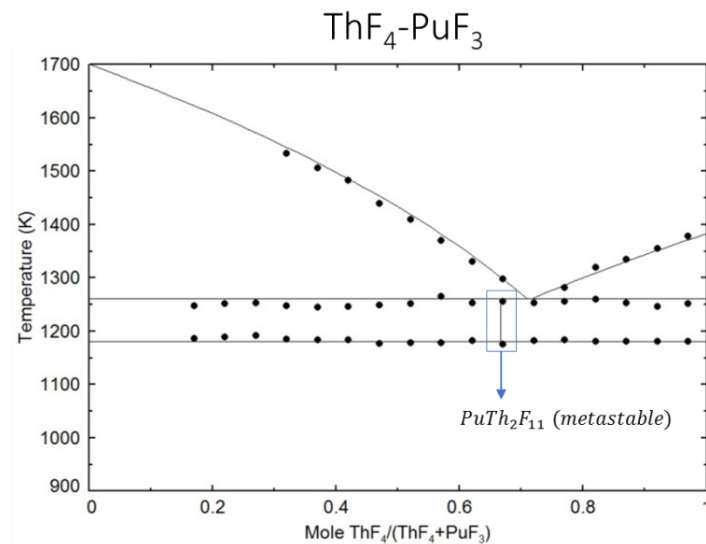


P. Souček, O. Beneš, [A. Tosolin](#), R.J.M. Konings, *Chemistry of Molten Salt Reactor Fuel Salt Candidates*, Trans. Am. Nucl. Soc., 118 (2018) 114-117.

Highlights: New phase diagrams



A. Tosolin, P. Souček, O. Beneš, J.-F. Vigier, L. Luzzi, R.J.M. Konings, *Synthesis of plutonium trifluoride by hydro-fluorination and novel thermodynamic data for the PuF₃-LiF system*, J. Nucl. Mat. 503 (2018) 171-177.

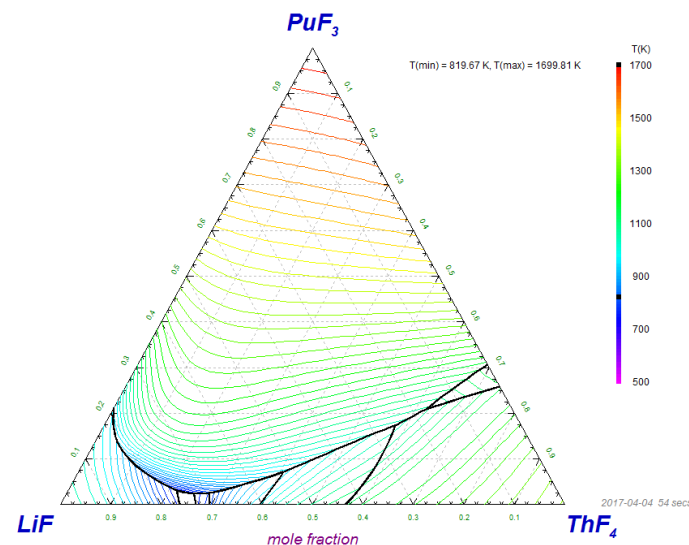


A. Tosolin, S. Mastromarino, J.-F. Vigier, L. Luzzi, R.J.M. Konings, O. Beneš, *Phase transitions in the ThF₄-PuF₃ system*, in preparation.

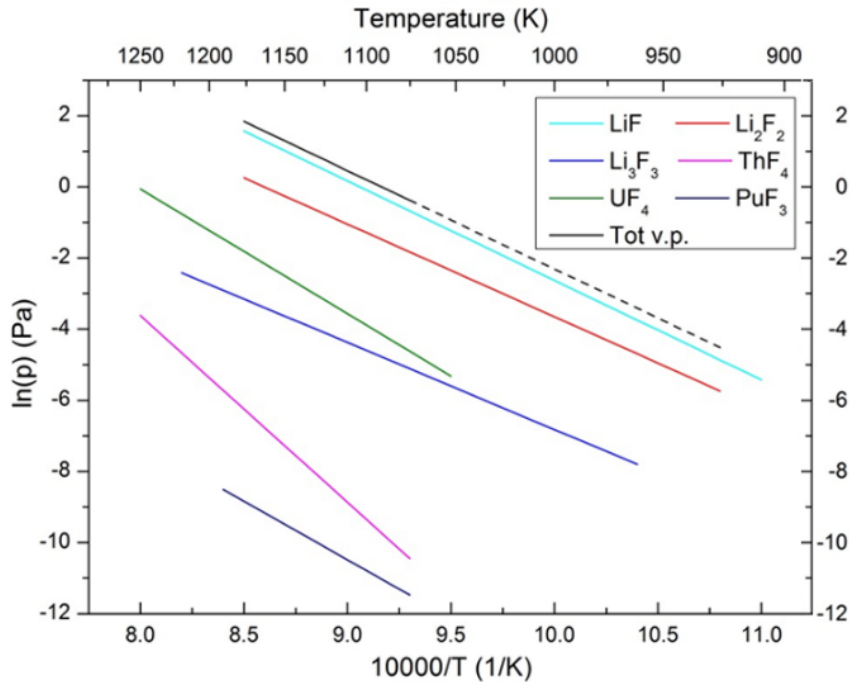


Improved thermodynamic database: JRCMSD

- fuel optimization
- properties prediction



Highlights: Properties of MSFR selected fuel compositions



LiF-ThF₄-UF₄
(77.5-20.0-2.5 mol%)

T_m (by DSC) = 828 ± 3 K

T_b = 2019 ± 10 K

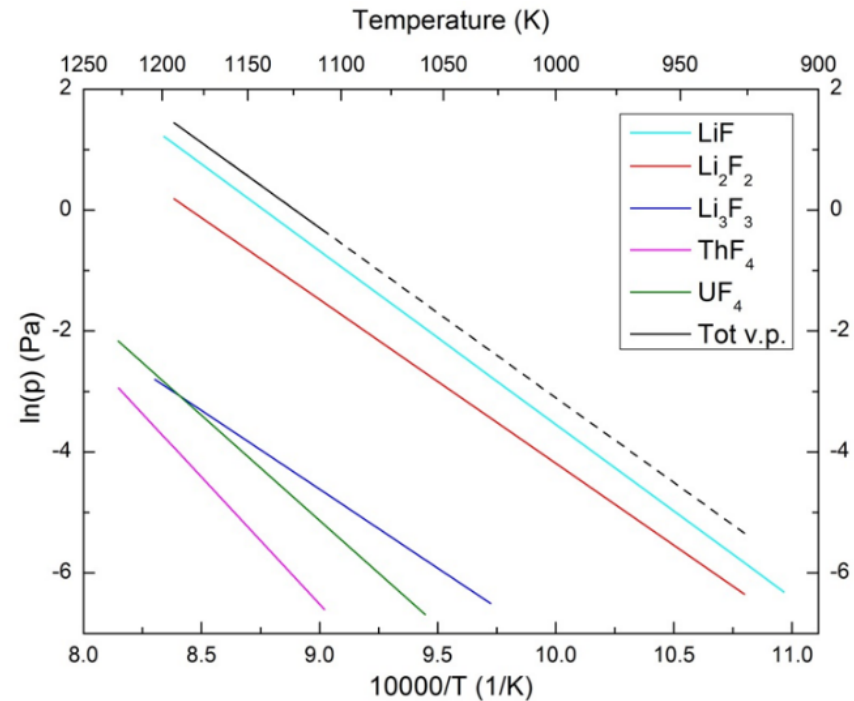
$v.p.$ (1000 K) = 0.045 Pa \pm 50%

LiF-ThF₄-UF₄-PuF₃
(77.5-6.6-12.3-3.6 mol%)

T_m (by DSC) = 893 ± 5 K

T_b = 1908 ± 10 K

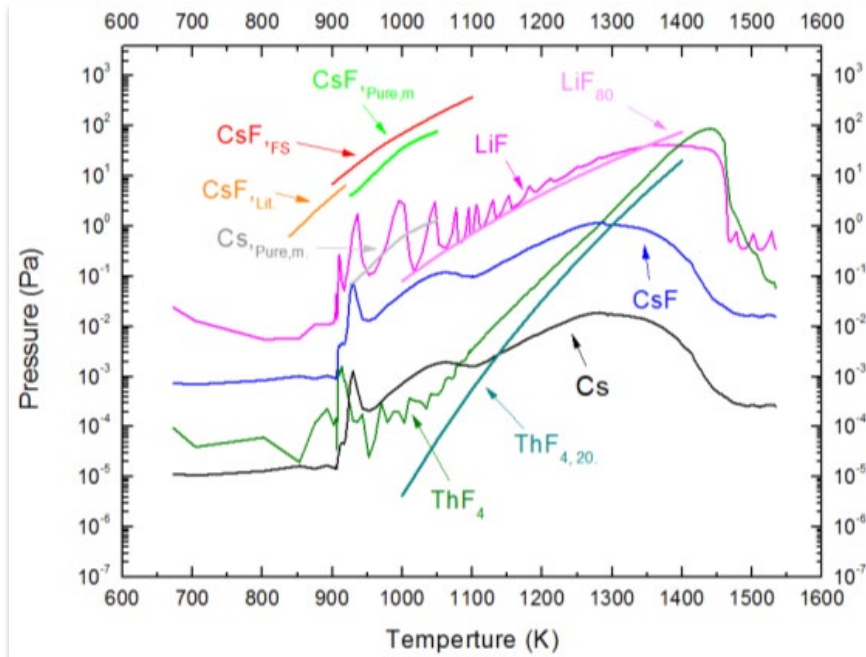
$v.p.$ (1000 K) = 0.099 Pa \pm 50%



Highlights: Retention of Cs in the MSR fuel

- to demonstrate retention of FP in the fuel matrix
- to determine volatility of the fuel
- to determine thermodynamic stability
- to determine gas composition

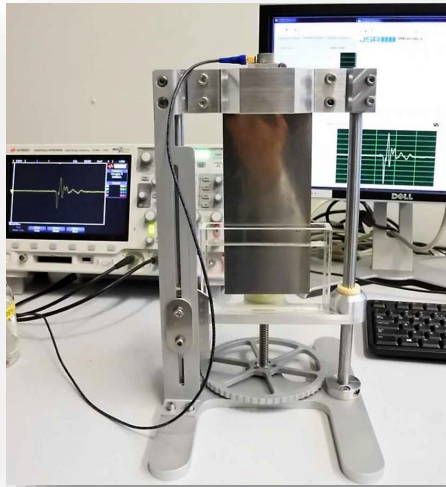
CsF dissolved in LiF - ThF₄



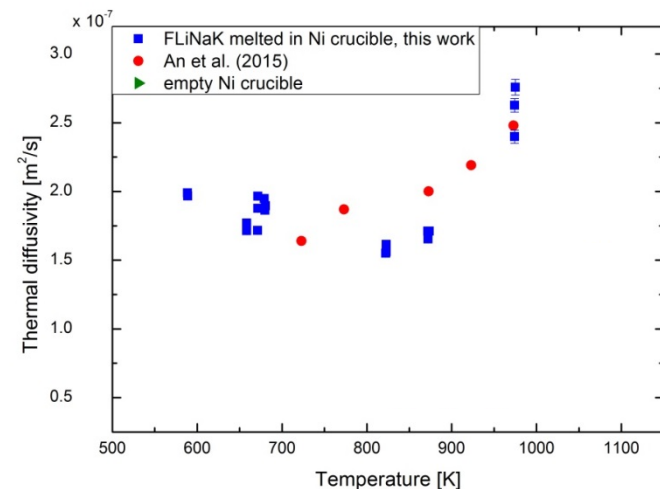
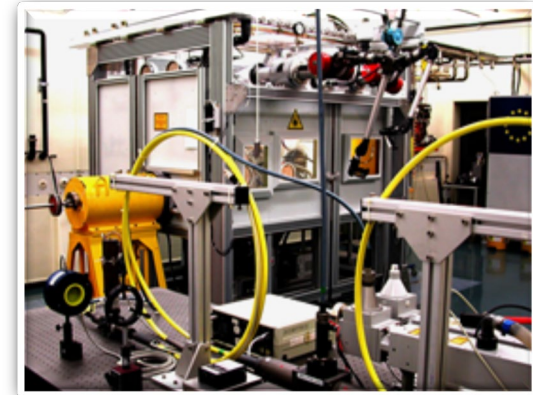
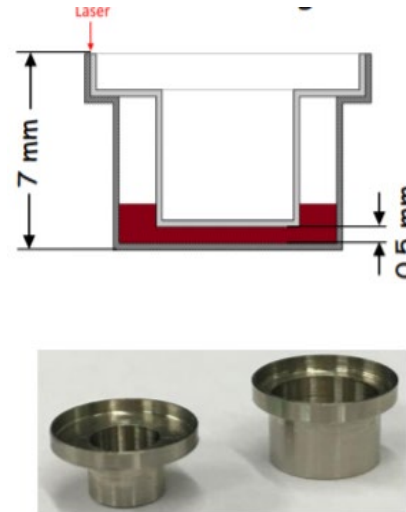
CsF is one of the stable form of Cs-FP in the MSR fuel:



Highlights: Development of New Experimental techniques

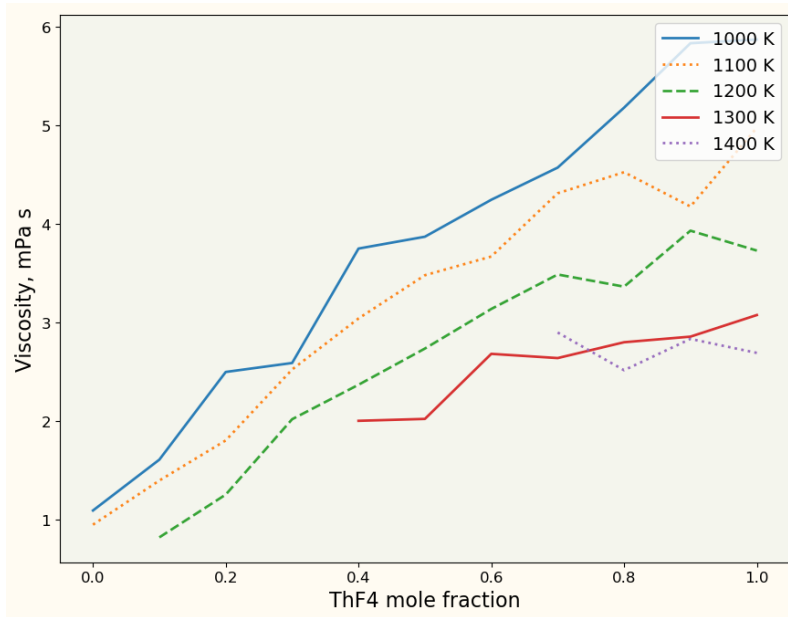


Fluid	T	Viscosity ultrasound	relative error to real value
	°C	mPa s	%
Water	26.3 ± 0.07	0.78 ± 0.03	0.26
	25.1 ± 0.07	0.85 ± 0.03	6.3
	25.3 ± 0.11	0.87 ± 0.02	6.7
96% Ethanol	26.3 ± 0.1	1.07 ± 0.01	–
	26.2 ± 0.04	1.19 ± 0.01	1.6
Oil	27.8 ± 0.24	42 ± 0.66	5.1
	27.8 ± 0.17	42.4 ± 0.43	6.1
Water/Glycerine 30/70 vol %	27.7 ± 0.07	20.6 ± 0.16	5.5
	26.8 ± 0.56	21.1 ± 0.9	4.6
ionic salt	27.4 ± 0.22	17.55 ± 0.43	22.5
	28.0 ± 0.11	16.88 ± 0.17	24.9

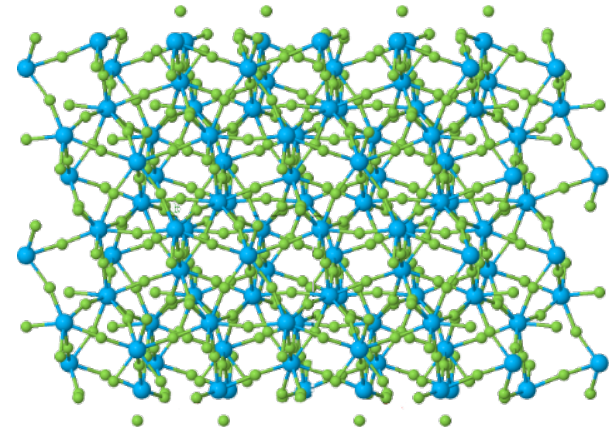


Highlights: Molecular Dynamics

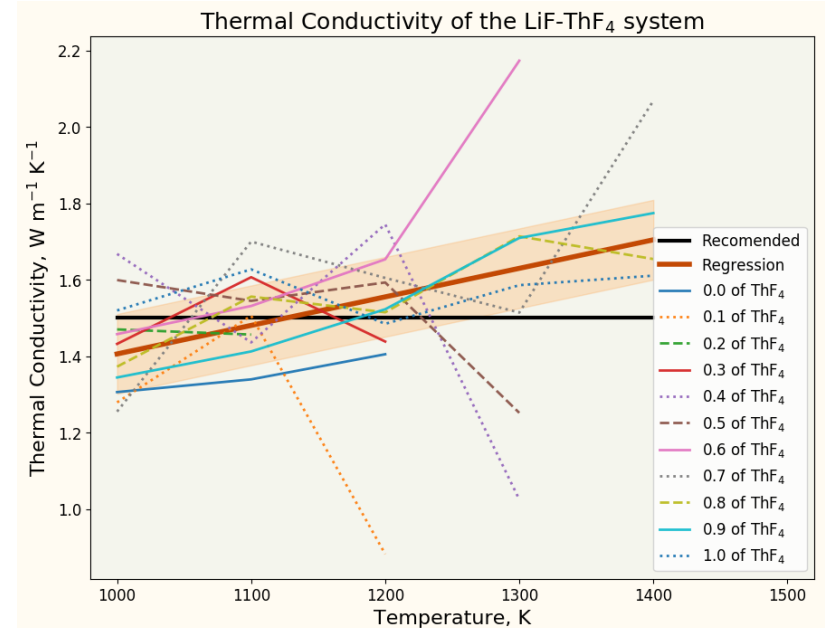
Calculated viscosity of LiF-ThF₄ system as a function of composition



Structure of ThF₄



Thermal conductivity of LiF-ThF₄ system as a function of temperature



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Total scientific output up to date:

- 2 / 2 Milestones Achieved
- 6 / 8 Deliverables Done
- 3 Peer review articles Published (2 by Alberto lead)
- 2 Papers in press – to be submitted within 1 month (2 Alberto lead, 2 Sara co-author)
- 3 Papers to be submitted by the end of 2019 (1 Alberto lead, 1 Sara lead)
- ... and of course 2 PhD students granted with great output and effort

Stay in touch



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Task 2.1 – Thermodynamic data of salts

- Synthesis of UF_4 , ThF_4 and PuF_3 done
 - Re-evaluation of UF_4 melting point done
 - Phase diagram on LiF-PuF_3 done
 - $\text{ThF}_4\text{-PuF}_3$ is finalized (**Publication drafted** by Alberto, additional help by Sara)
- } → **Published in JFC 200 (2017) 3340**
- **Published in JNM 503 (2018) 171**
- Delivered (D2.1)**

Task 2.2 – Thermal properties of salts

- viscometer under development – construction and testing ongoing
- heat capacity of ThF_4 and LiF-ThF_4 measured (interpretation phase) → **Publication in press**(Alberto presentation)
- melting point determination of Option 1 (**Published in JNM 508 (2018) 319**) and Option 2 **done** (Alberto & Sara presentation) (**Publication in press**),
- thermal conductivity – crucible design done with first tests on LiF (presentation Alberto)
- viscosity will follow
- MD simulations

Task 2.3 – Phase segregation of salts

- estimations of primary crystallization phases have been done for both fuel compositions
- final results done and **Delivered (D2.3)**

Task 2.4 – Thermal conductivity of solid crust

- Being developed and measured – according to plan. Tests on LiF and PuF_3 done (Sara presentation).

Task 2.5 – Salt interaction with water

- Measurements being performed at TUD with and W/O Co-source **Delivered (D2.5)**
Publication in preparation

Task 2.6 – Retention properties of elements in the fuel salt

- KEMS measurements with LiF- UF_4 - ThF_4 salts containing Cs and I done
- supported by Thermodynamic modelling – Done and **Delivered (D2.2), Publication in Preparation**
- Te study with respect to redox potential – done by CNRS and **Delivered (D2.4)**

Task 2.7 – Vaporization behaviour under accidental conditions

- KEMS measurements of Option 1 and 2 compositions **Delivered (D2.3)**
(Option 1: Published in *JNM 508 (2018) 319*, Option 2: Paper in press)

(Alberto presentation)

- Aerosol particle distribution simulated with and without LiF influence **Delivered (D2.6)**