SAM SAFER

WP2 Experiments and Simulations on MSR fuel systems

Final Project meeting

Avignon

28.11.2023

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3 Keynote Lectures

Nikolas Scuro – PhD Student of Ontario Tech., with stays at Polimi at JRC (Remote presentation)
Coupling of Thermodynamics with Multi-physics – Fluorination and overheating scenario

Thomas Dumaire – PhD Student of TUD, with work at JRC
Thermodynamics of Fuel Salt with corrosion products – Experiments and Simulations

Stefano Lorenzi – Professor at Polimi
Multi-Physics simulations with focus on 5M particle dynamics

OntarioTech Engineering & Applied Science

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WP2 - Task 2.1
Final Results Coupling OpenFOAM and Thermochimica for MSR

Final Meeting & Exploitation Workshop
November 28-30, 2023, Avignon, France

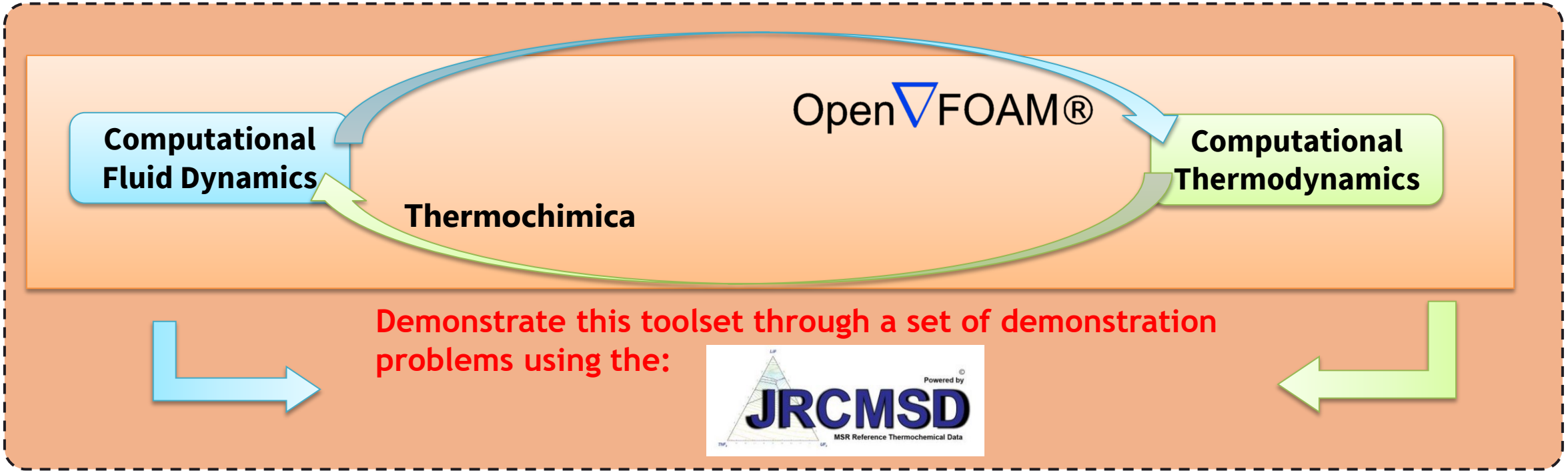
N. L. Scuro, O. Beneš, M. H. A. Piro

Outline

- ❑ **WP2 - Task 2.1**
- ❑ **Coupling Method**
- ❑ **Two-Way Coupling Demonstration Problems (#1 and #2)**
- ❑ **Verification and Validation (V&V)**
- ❑ **Conclusions**
- ❑ **Acknowledgments**

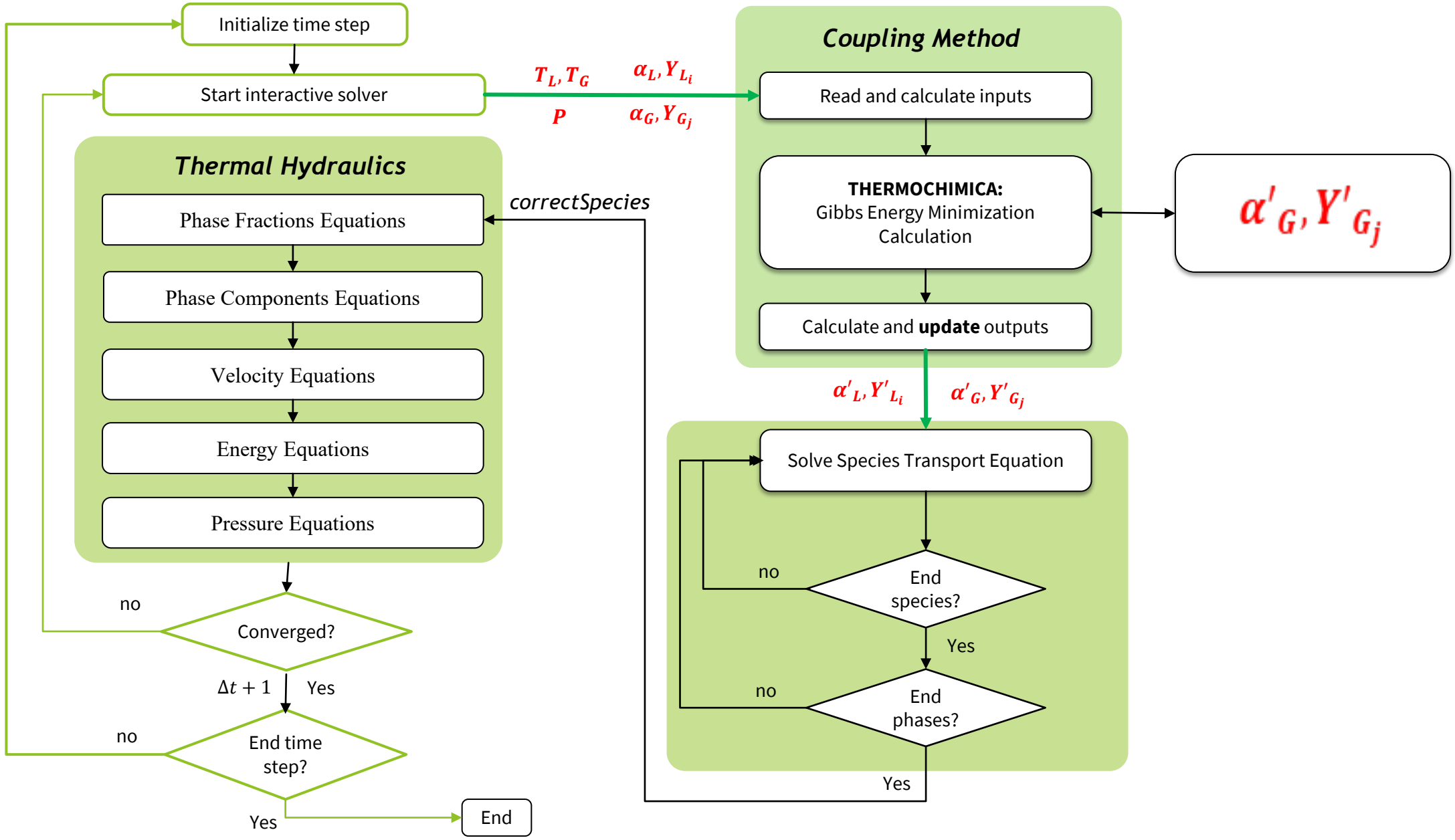
WP2 - Task 2.1

"To develop new **computational capabilities** to simulate **phase transformations** and **chemically reacting dynamic flows** involving **molten salts**"



Note: This project is **not** a predictive tool for industry… **Yet!**

Coupling Method

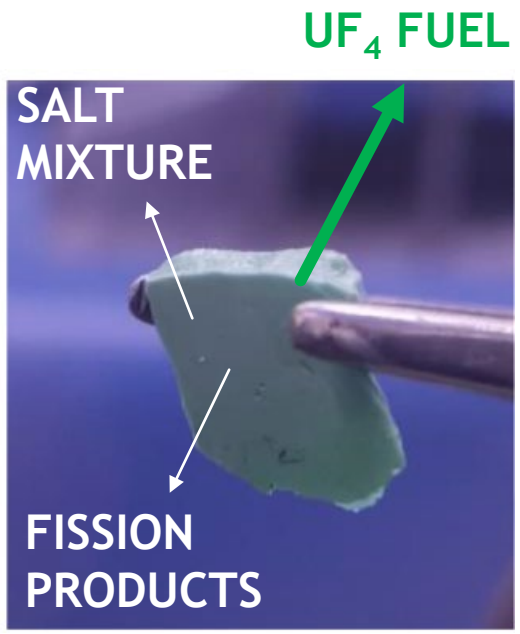


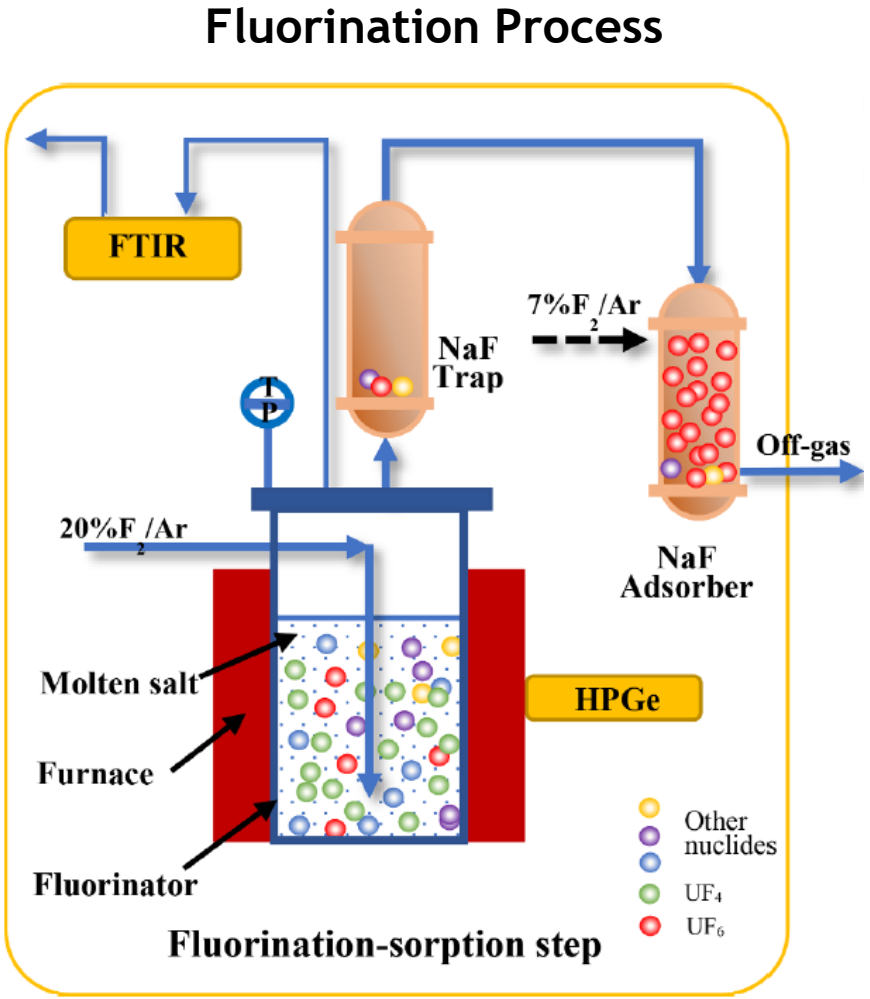
1st Demonstration Problem

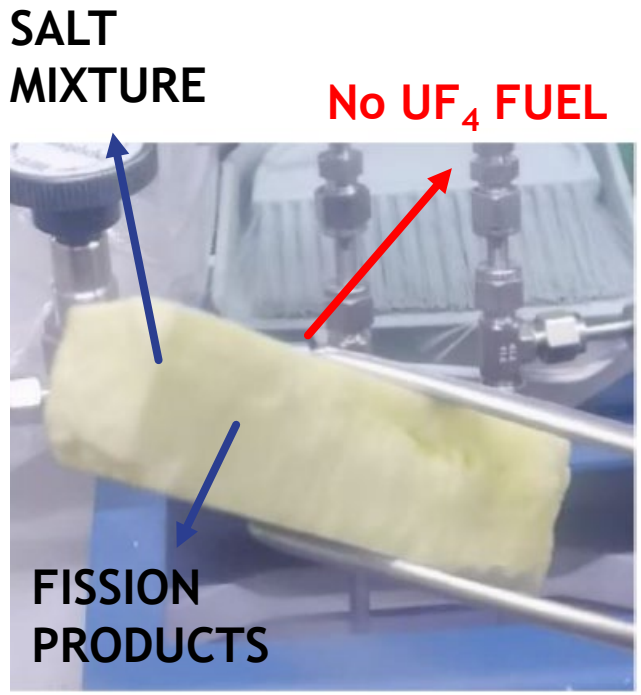
Fluorination Process

$$UF_4 + F_2 \rightarrow UF_6$$

Demonstration Problem: Molten Salt Fluorination Process ($UF_4 + F_2 \rightarrow UF_6$)

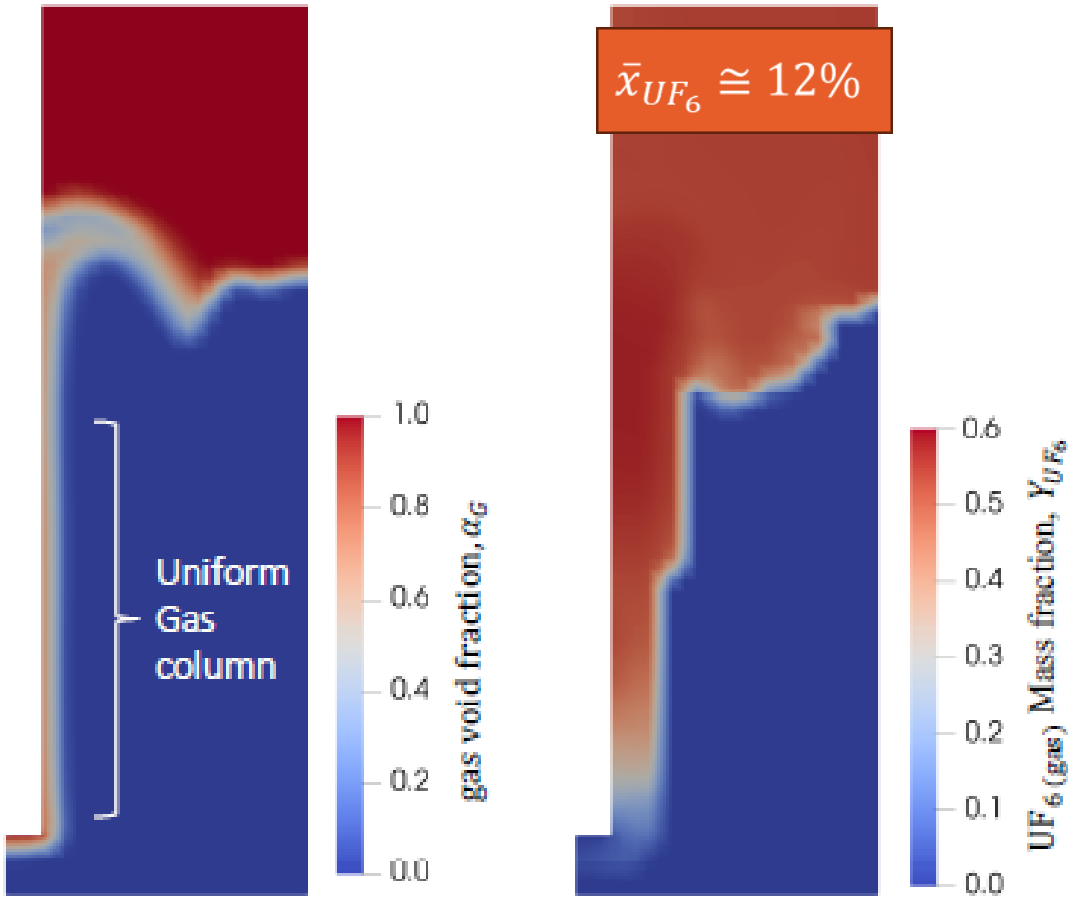






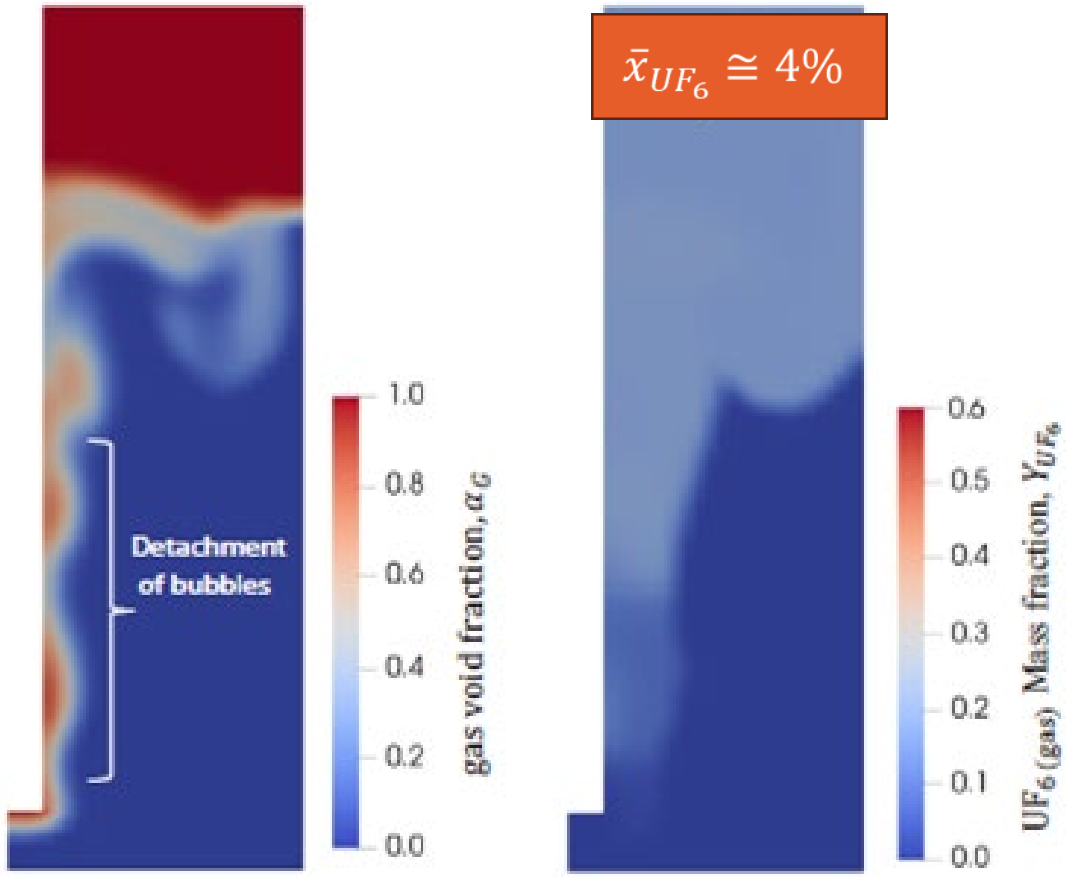
Qiang Dou and Qingnuan Li et al. (2022). Journal of Fluorine Chemistry, 261, 110016.

Demonstration Problem: Molten Salt Fluorination Process ($UF_4 + F_2 \rightarrow UF_6$)



Case 1: lowest viscosity

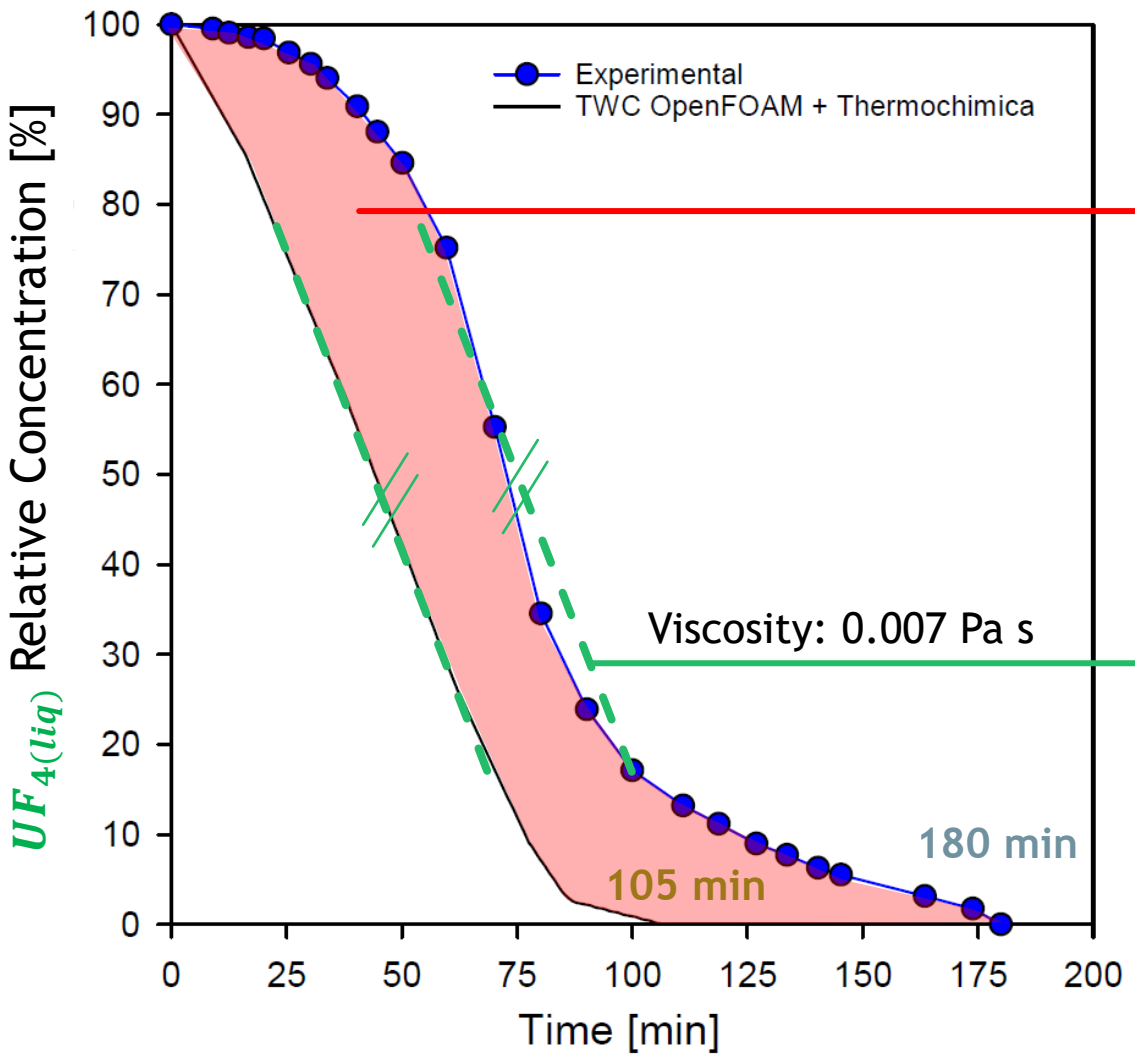
Fluorination time: 105 min



Case 1: Highest viscosity

Fluorination time: 663 min

#2 TWC Demonstration Problem: UF_4 removal rate



Difference between TWC vs Experimental :c

1. Lack of chemical kinetics
2. Lack of chemical and temperature dependencies of thermophysical properties
3. Several uncertainties from experiments results

Very similar reaction rates at Steady-State

N.L. Scuro, O. Benes, M.H.A. Piro, *"Two-Way Coupling of OpenFOAM and Thermochimica for Fluoride Volatility Processes in Molten Salt Reactor Applications"* [Under Review by Annals of Nuclear Energy], (2023).

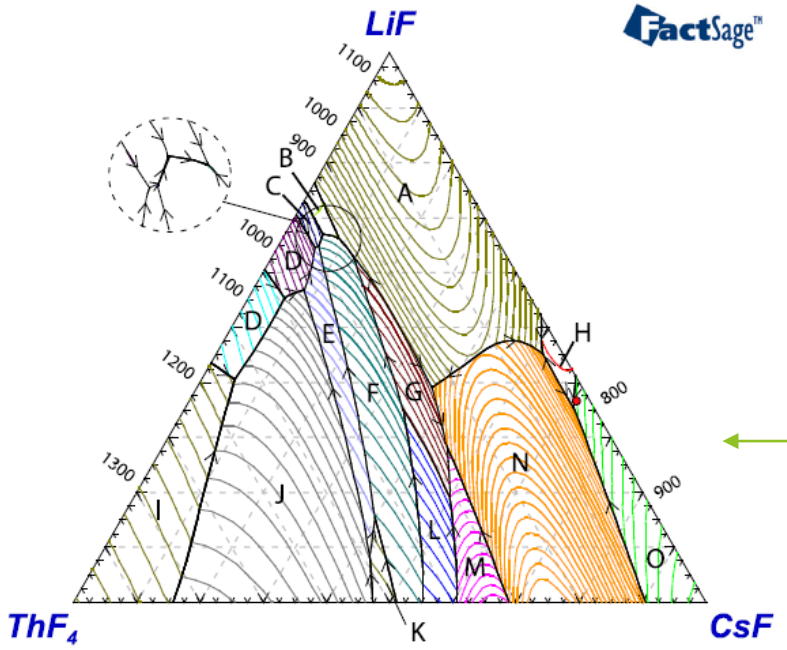
2nd Demonstration Problem:

Molten Salt Fast Reactor

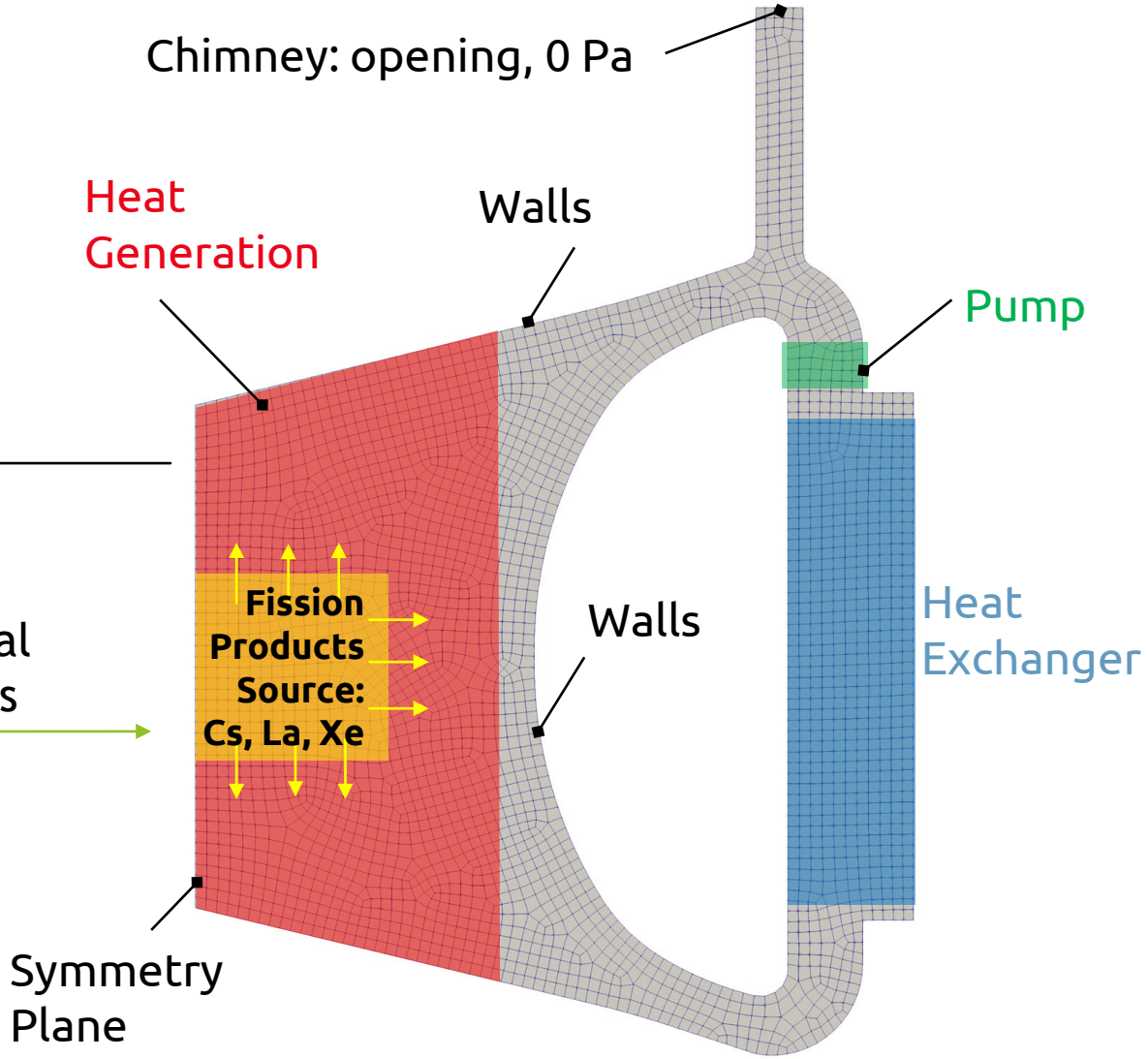
Normal Operation Conditions and Overheating Scenarios

2nd Demonstration Problem - Molten Salt Fast Reactor

Salt: LiF-ThF_4-UF_4
77.5-20.0-2.5 %mol.

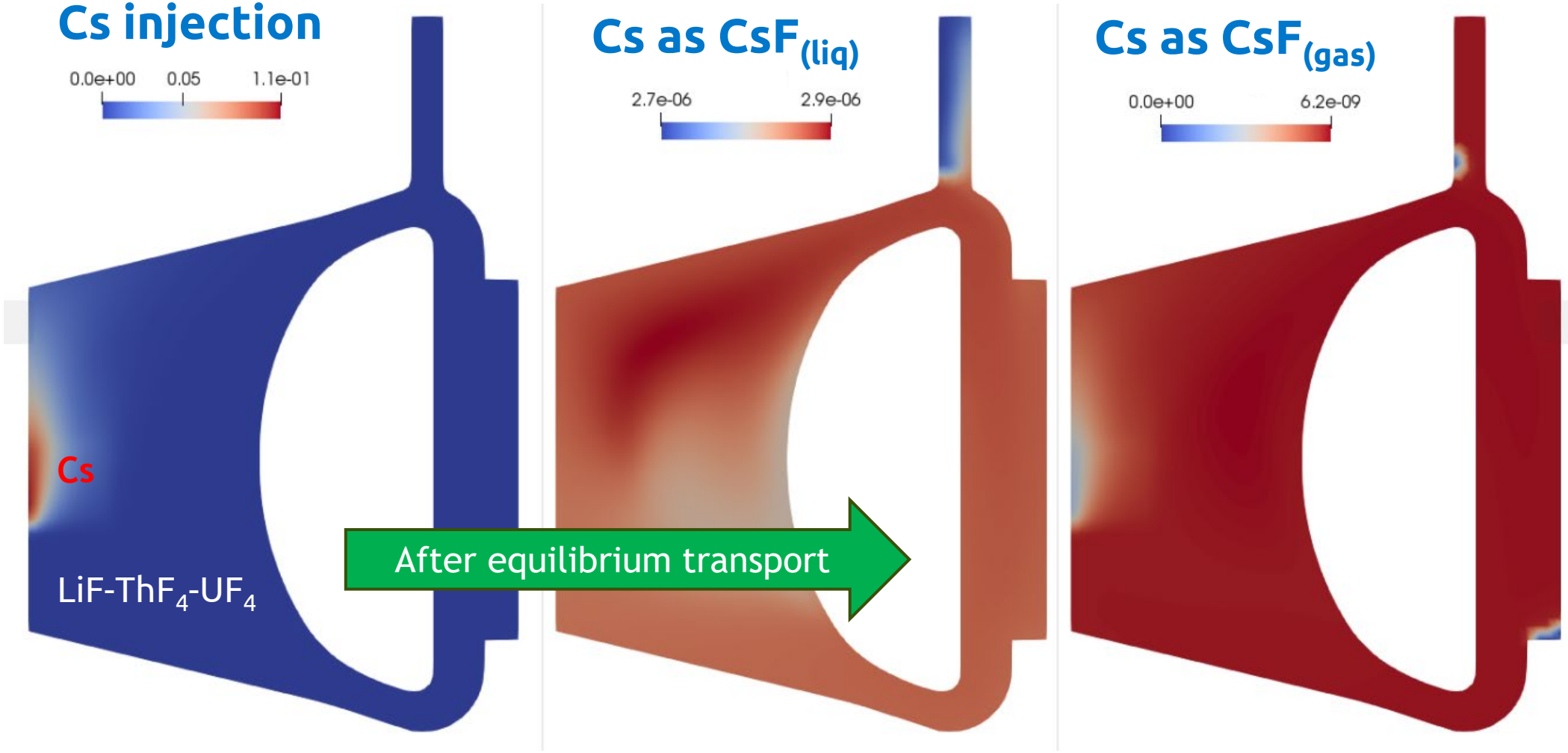


Non ideal solutions



Capelli, E., Beneš, O., & Konings, R. J. M. (2018). *Journal of Nuclear Materials*, *501*, 238-252.

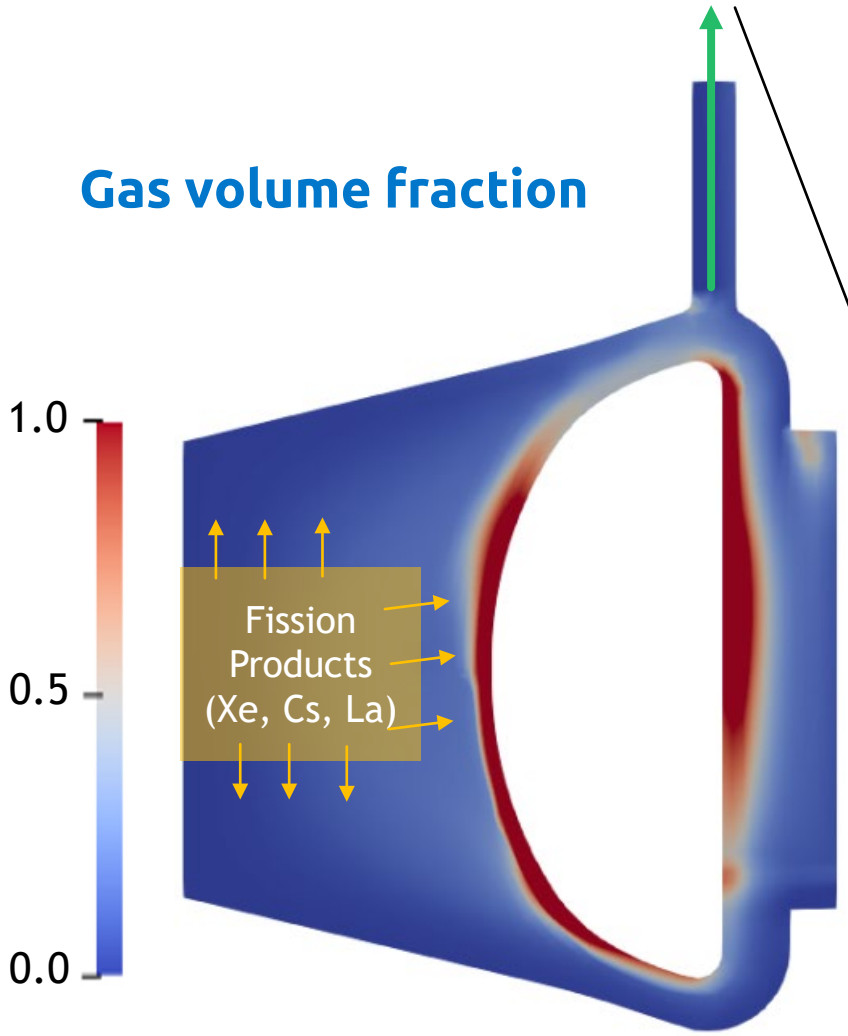
2nd Demonstration Problem - Molten Salt Fast Reactor



N. L. Scuro, O. Beneš, S. Lorenzi, M. Krstovic, S. Krepel, M.H.A. Piro (under review).

2nd Demonstration Problem - Molten Salt Fast Reactor

Gas volume fraction

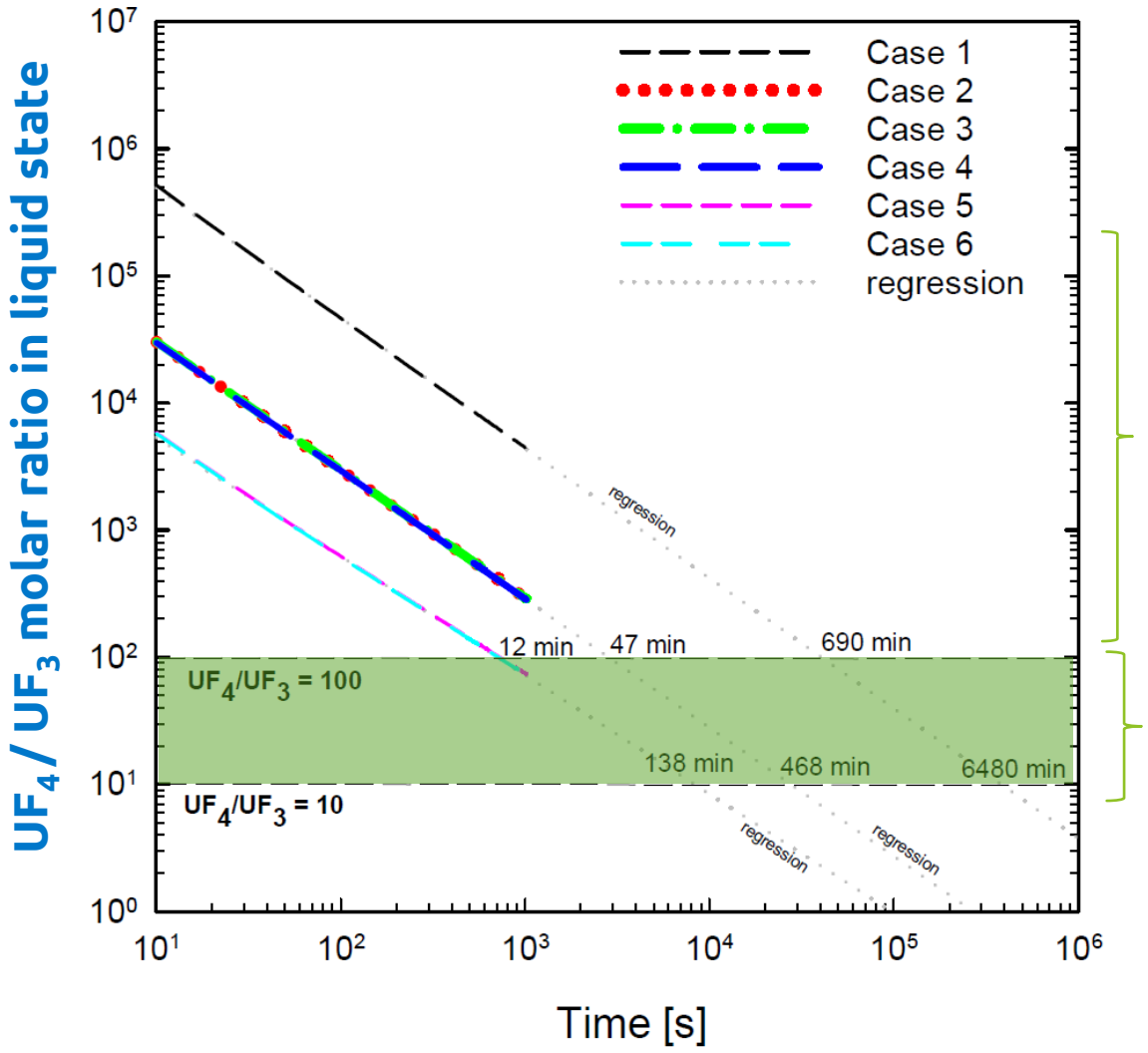


Gaseous Species accumulated in 1000 s

Species [kg]	NOC 3 GW_{th}	Overheating 15 GW_{th}
Xe	1.011E-05	5.056E-05
FLi	1.311E-11	9.029E-08
F2Li2	5.146E-12	2.310E-08
F3Li3	7.686E-13	3.045E-09
ThF4	1.149E-13	8.338E-09
UF4	2.962E-13	5.667E-09
UF3	1.148E-19	2.124E-13
CsF	1.444E-12	2.140E-09
Cs2F2	8.957E-17	2.007E-13
Cs2	1.463E-27	2.507E-21
LaF3	2.296E-18	1.266E-12
F2	1.032E-36	4.676E-26
F	2.449E-22	1.892E-15

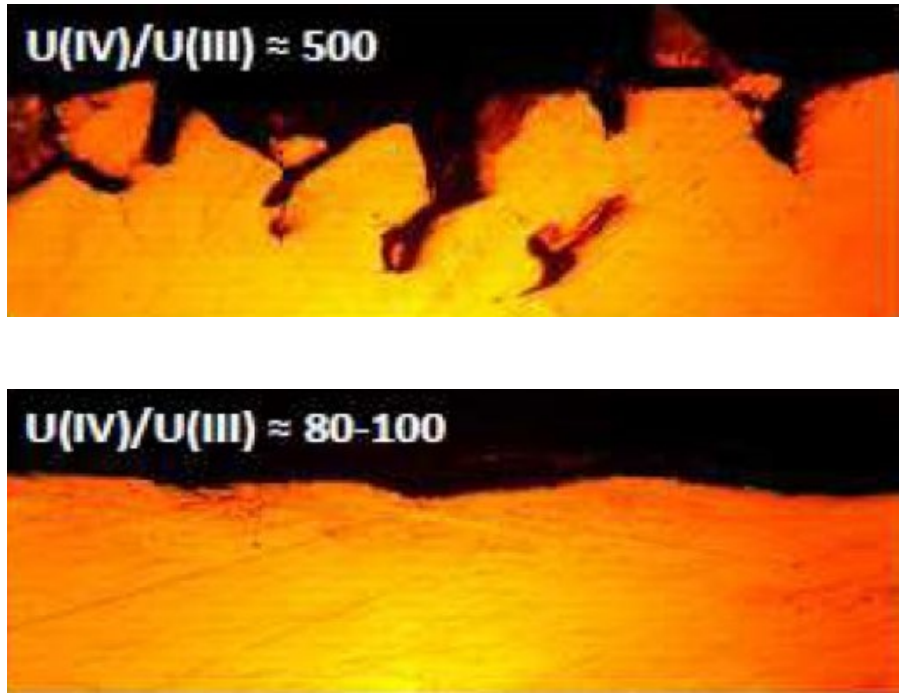
N. L. Scuro, O. Beneš, S. Lorenzi, M. Krstovic, S. Krepel, M.H.A. Piro (under review).

2nd Demonstration Problem - Molten Salt Fast Reactor



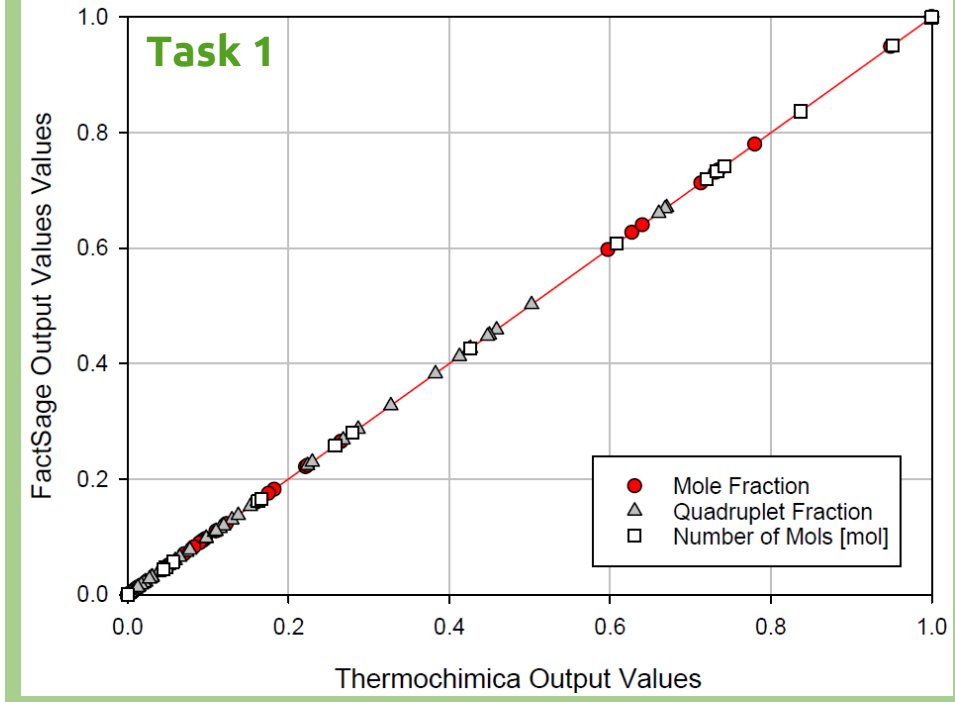
N. L. Scuro, O. Beneš, S. Lorenzi, M. Krstovic, S. Krepel, M.H.A. Piro (under review).

UF_4 / UF_3 : Corrosion Buffer



Final report summary – EVOL, Tech. Rep. Project n°249696, Centre national de la recherche scientifique (CNRS), 4, 2015.

Numerical Verification



- Benchmark report of Thermochimica vs FactSage™ for the SAMOSAFER was made in Fall 2021*

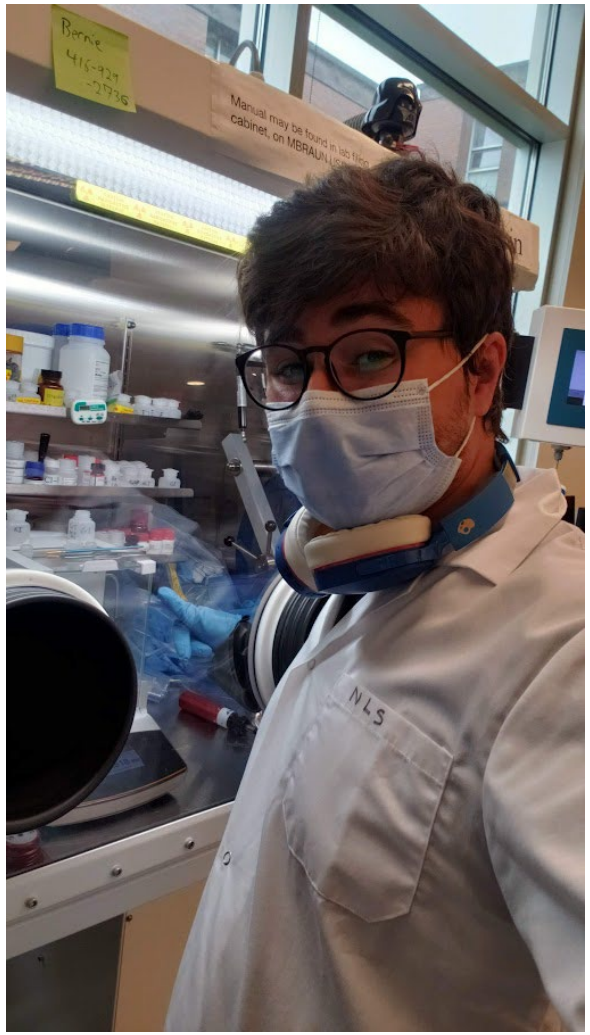
- CFD model itself follows the best guidelines[1,2] to achieve numerical convergence (mesh sensitivity, track residuals, appropriate numerical schemes, turbulence model, etc.)

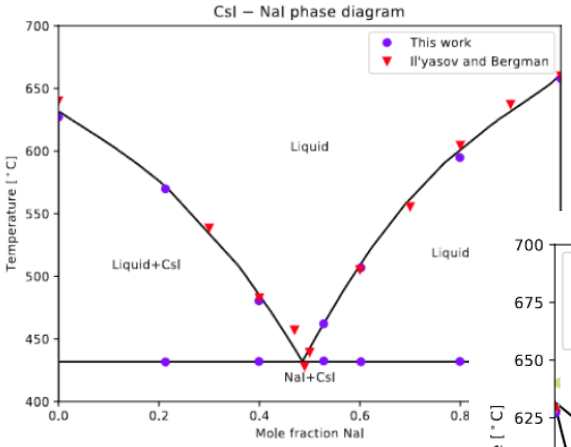
* **N. L. Scuro**, *et al*, (2023) "D2.2 – Description of thermodynamic database implemented in Thermochimica", SAMOSAFER, EURATOM, 847527

[1] Oberkampf, W. L., & Trucano, T. G. (2002). Verification and validation in CFD. *Progress in aerospace sciences*, *38* (3), 209-272

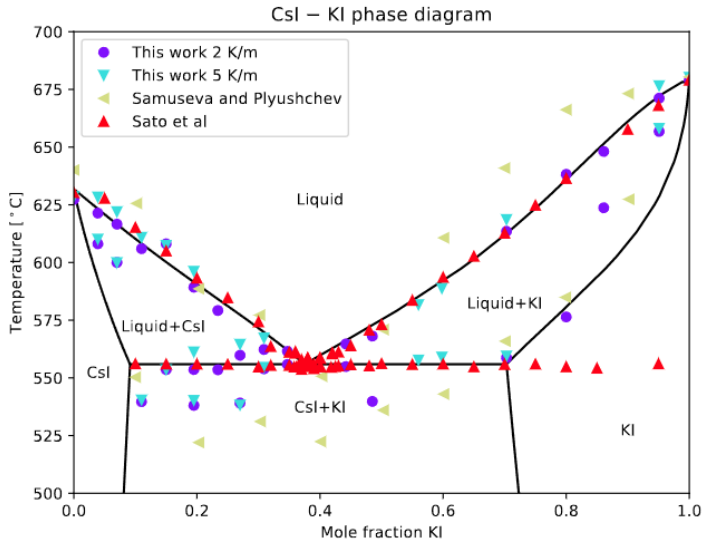
[2] Mahaffy, J. *et. al* (2015). No. NEA-CSNI-R--2014-11, OECD

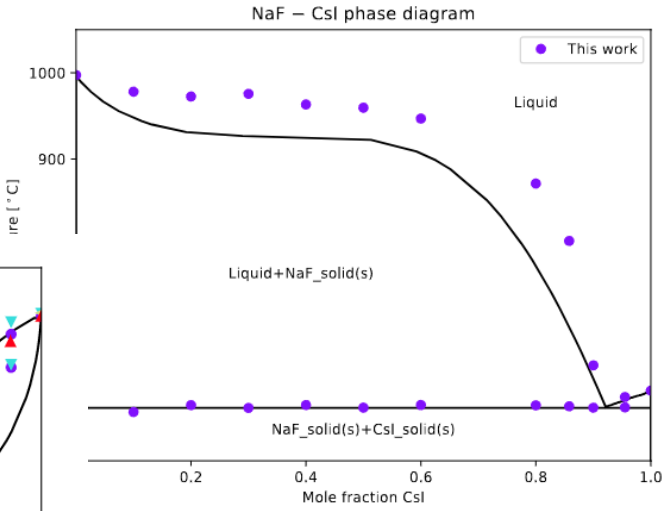
Numerical Validation





Corroborated by JRC





N.L. Scuro et al. *"Thermodynamic investigations of the KI-CsI, NaI-CsI, NaF-CsI pseudo-binary systems"* [to-be-submitted]

- All thermodynamic calculations are based on experimental inputs.
- OTU has been corroborating with JRC on the development of salt systems:
- KI-CsI, CsI-NaI, NaI-CsI, NaF-CsI, KF-CsI, $MgCl_2$-$SrCl_2$

Conclusions

- Can provide **time required** for molten salt reactions (i.e., fluorination)
- Can provide **how thermophysical properties can affect reactions** (i.e., viscosity)
- Can provide **how much and and which rate fission products are retained or released**
- Can provide inputs for **UF4/UF3 corrosion buffer lost**

Acknowledgements

- This research was undertaken, in part, thanks to funding from the Canada Research Chairs program (950-231328) of the Natural Sciences and Engineering Research Council of Canada.

- To the SAMOSAFER project for the travel grant (SAMOSAFER Mobility Scheme) at PoliMi and JRC!

- I’d like to thank, A. Di Ronco (PoliMi), S. Lorenzi (PoliMi), T. Dumaire (JRC/TUD), O. Benes (JRC), Sophie Deanesi (PoliMi), Milica Krstovicfor (PSI) and Jiri Krepel (PSI) for technical discussions and support.

It was a pleasure to work at this project!

Questions and inputs are welcome!

nikolas.scuro@ontariotechu.net

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Thermodynamics of Fuel Salt with corrosion products – Experiments and Simulations

T. Dumaire, O. Beneš, O. Walter, R. Konings, A.L. Smith

Final Project meeting

Avignon

28.11.2023

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Outline

Corrosion studies

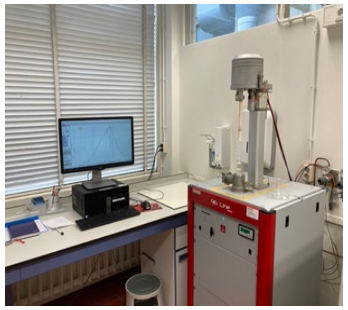
- Chemical speciation of Cr in molten salt
- $LiF\text{-}CrF_3$, $NaF\text{-}CrF_3$, $KF\text{-}CrF_3$ thermodynamic assessments
- $CrF_2\text{-}CrF_3$ thermodynamic assessment
- CrF_2 synthesis
- $LiF\text{-}CrF_2\text{-}ThF_4$ thermodynamic assessment

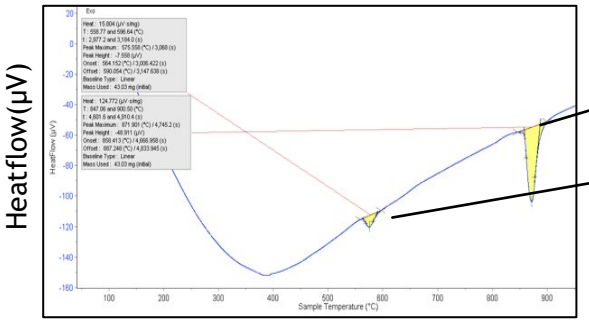
Fission products studies

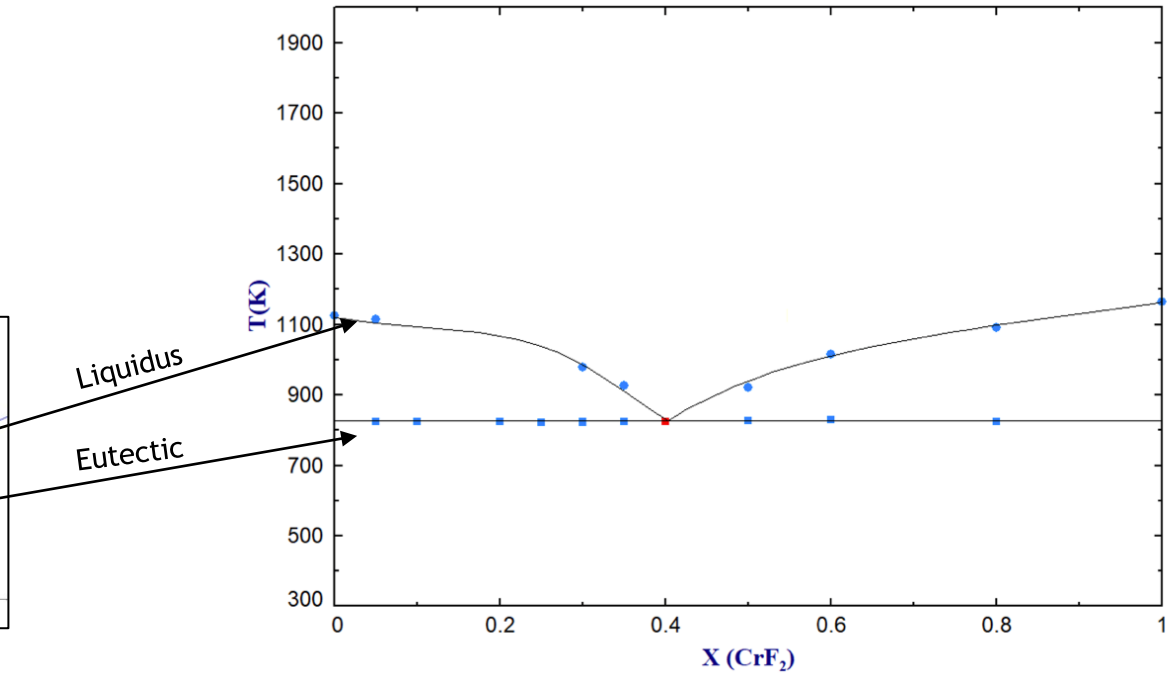
- Study case
- Impact on the fuel thermodynamical properties
- $LiF\text{-}BaF_2\text{-}ZrF_4$ thermodynamic assessment

Modeling method – Experimental data collection

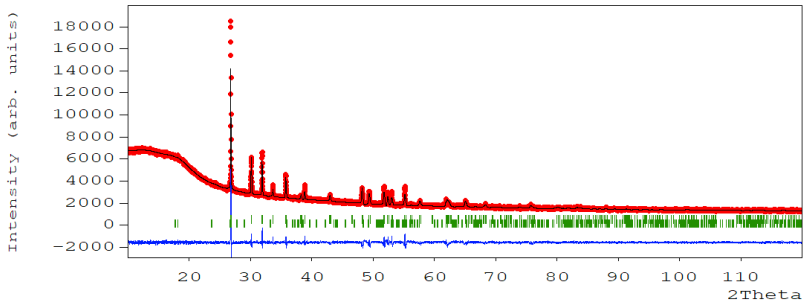
- Phase diagram measurements: Differential Scanning Calorimetry







- Phase identification: X-ray Diffraction



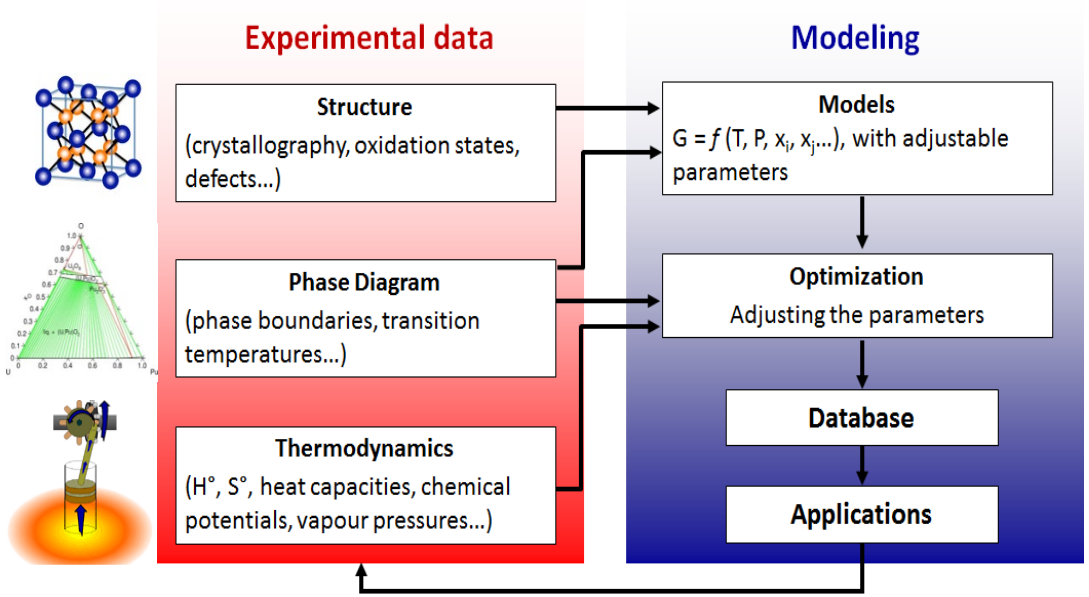
XRD spectra of the synthesized CrF_2 with a purity >99% determined by Rietveld refinement

LiF-NaF-KF-CrF_3 systems thermodynamic modeling

- CALPHAD

Least-square minimization of the total Gibbs energy G of the system to find the thermodynamic equilibrium at given conditions (T, P, xi).
G is expressed as a linear combination of the G for all phases:

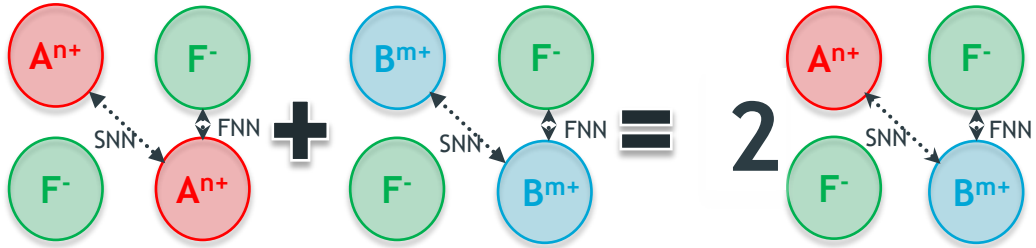
$$G(T,P,x_i) = \sum N^{\alpha}\, G_m^{\alpha}(T,P,x_i^{\alpha})$$



- **Modified quasichemical model in quadruplet approximation**
  - Formalism well-adapted to ionic liquids
  - Two sub-lattices

(A^{n+}, B^{m+}, cations, …) (F^-, Cl^-, anions)

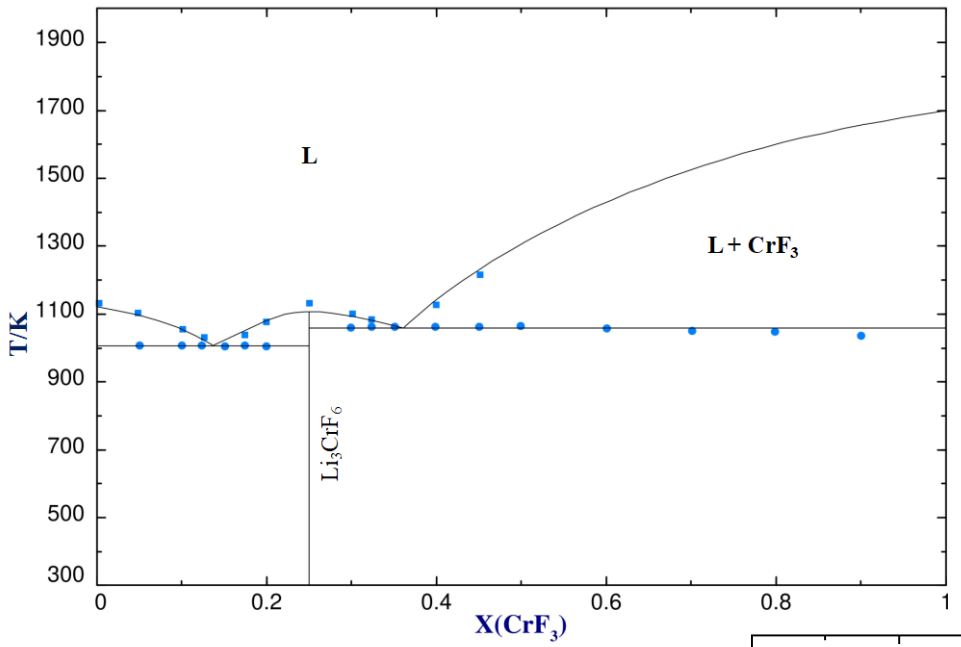
  - Basic unit = quadruplet composed of 2 anions and 2 cations



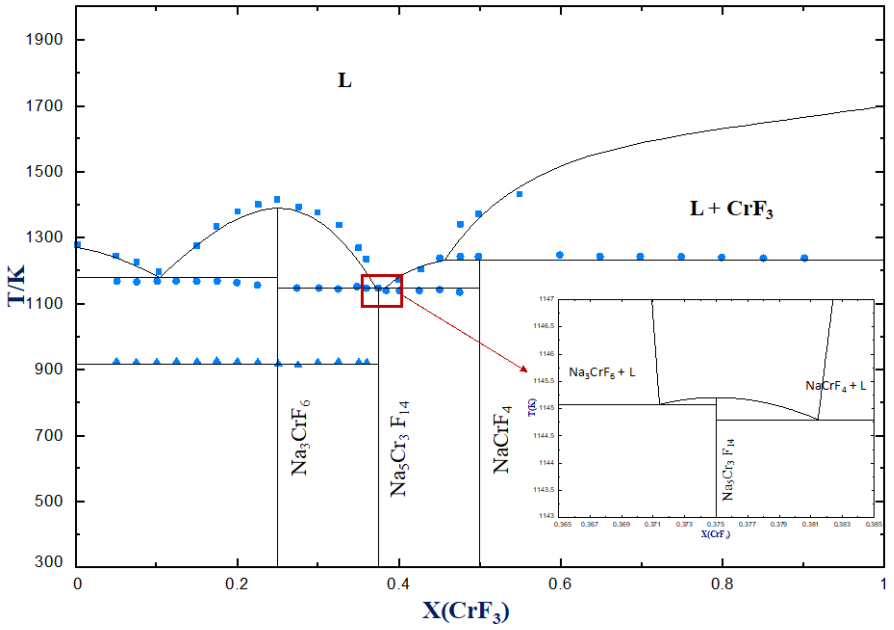
- Optimized excess parameters linked to SNN exchange reaction

$$\Delta g_{AB/F} = \Delta g^{0}_{AB/F} + \sum_{i\geq 1} g^{i0}_{AB/F}\, \chi^{i}_{AB/F} + \sum_{j\geq 1} g^{j0}_{AB/F}\, \chi^{j}_{AB/F}$$

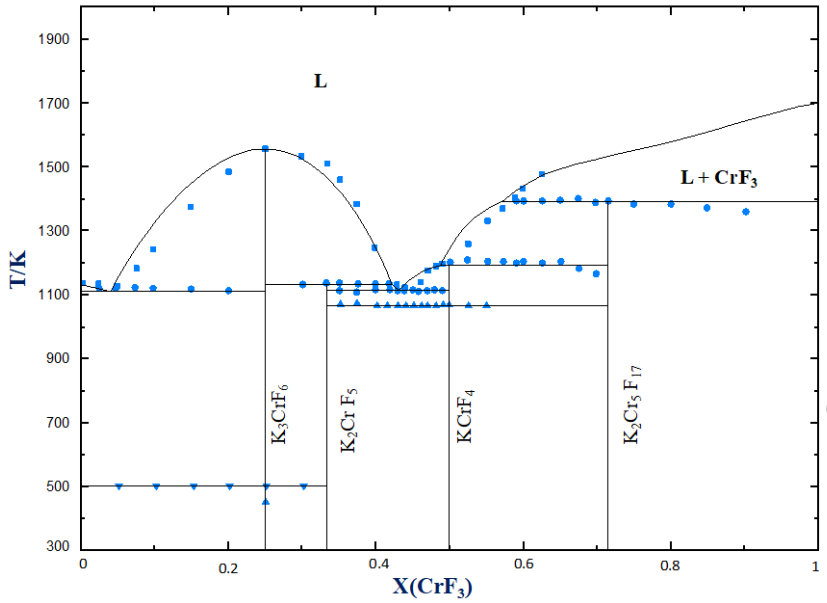
LiF-NaF-KF-CrF_3 systems thermodynamic modeling



CALPHAD modeling of the LiF-CrF_3 system



CALPHAD modeling of the NaF-CrF_3 system



CALPHAD modeling of the KF-CrF_3 system

[1] Dumaire, T., Konings, R. J., & Smith, A. L. (2021). Thermodynamic Assessment of the AF–CrF_3 (A= Li, Na, K) and CrF_2–CrF_3 Systems. Thermo, 1(2), 205-219

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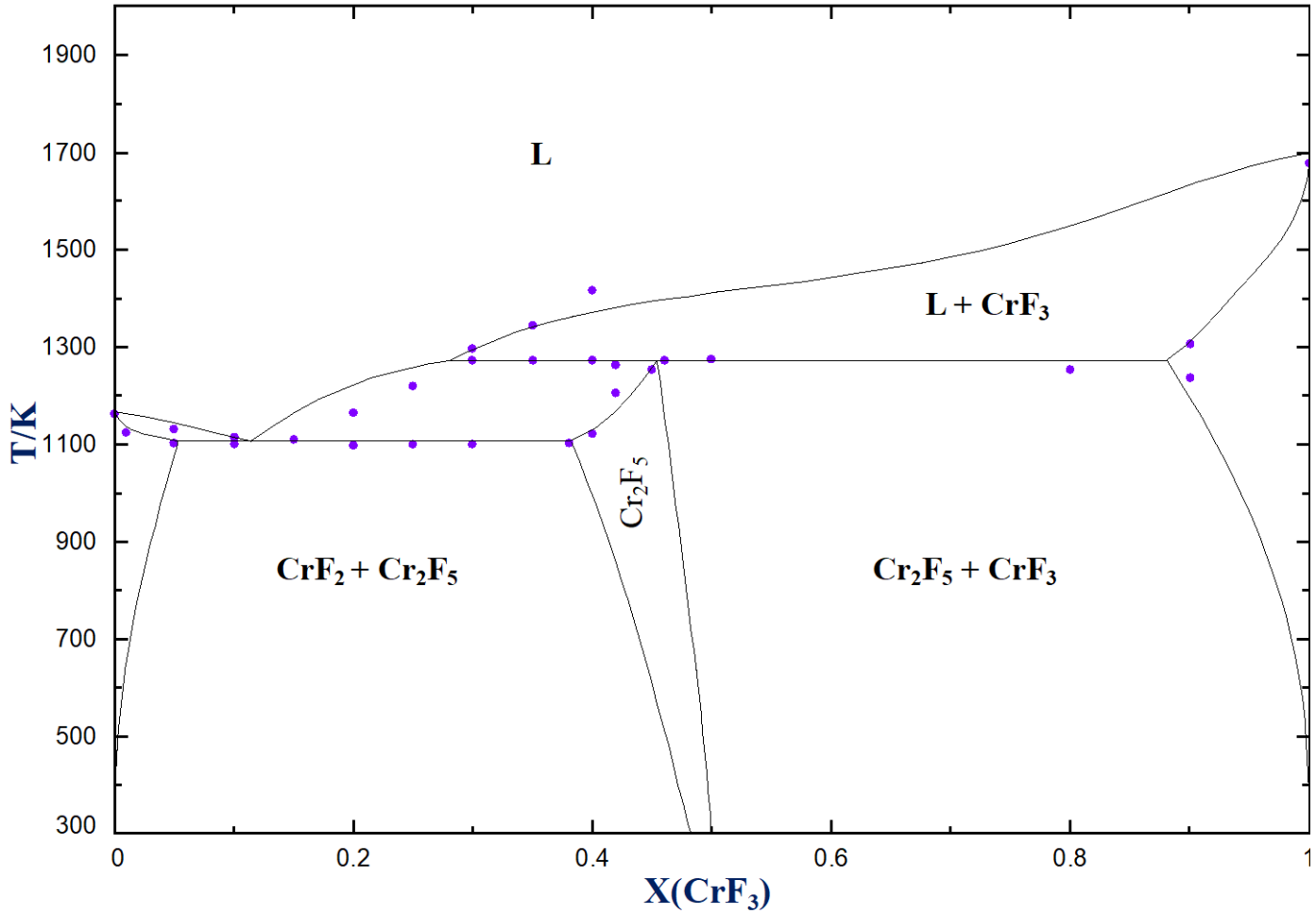
CrF_2-CrF_3 system thermodynamic modeling



CALPHAD modeling of the CrF_2-CrF_3 system

- System highly instable in Molten Salt Conditions
- CrF_3 likely to decrease in CrF_2 [1]

[1] Dumaire, T., Konings, R. J., & Smith, A. L. (2021). Thermodynamic Assessment of the AF-CrF_3 (A= Li, Na, K) and CrF_2-CrF_3 Systems. Thermo, 1(2), 205-219

Synthesis of CrF_2

$$2\ Cr_{(s)} + 4\ CH_3COOH_{(aq)} \rightarrow Cr_2(COOCH_3)_{4\ (s)}$$

$$Cr_2(COOCH_3)_{4\ (s)}\ (H_2O)_{(aq)} + 3\ NH_{3(aq)} + 6\ HF_{(aq)} \rightarrow 2\ NH_4CrF_{3\ (s)} + [\ldots]_{(aq)}$$

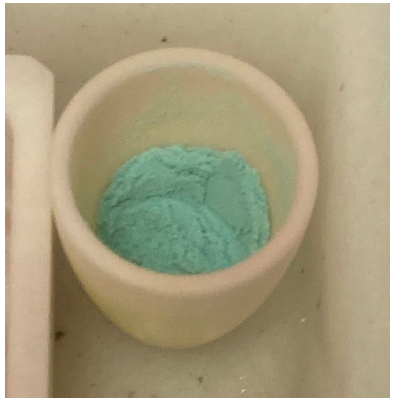
$$NH_4CrF_{3\ (s)} \rightarrow CrF_{2\ (s)} + NH_{3(g)} + HF_{(g)}$$

Ar, 873 K, 1h

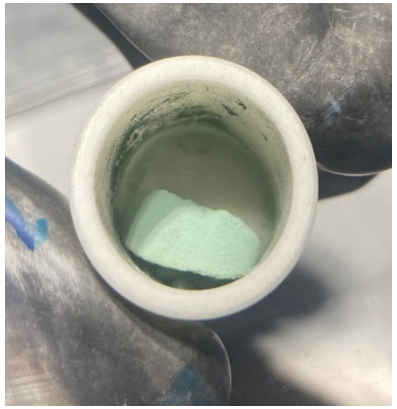
Chromium powder

$Cr_2(COOCH_3)_4$

NH_4CrF_3

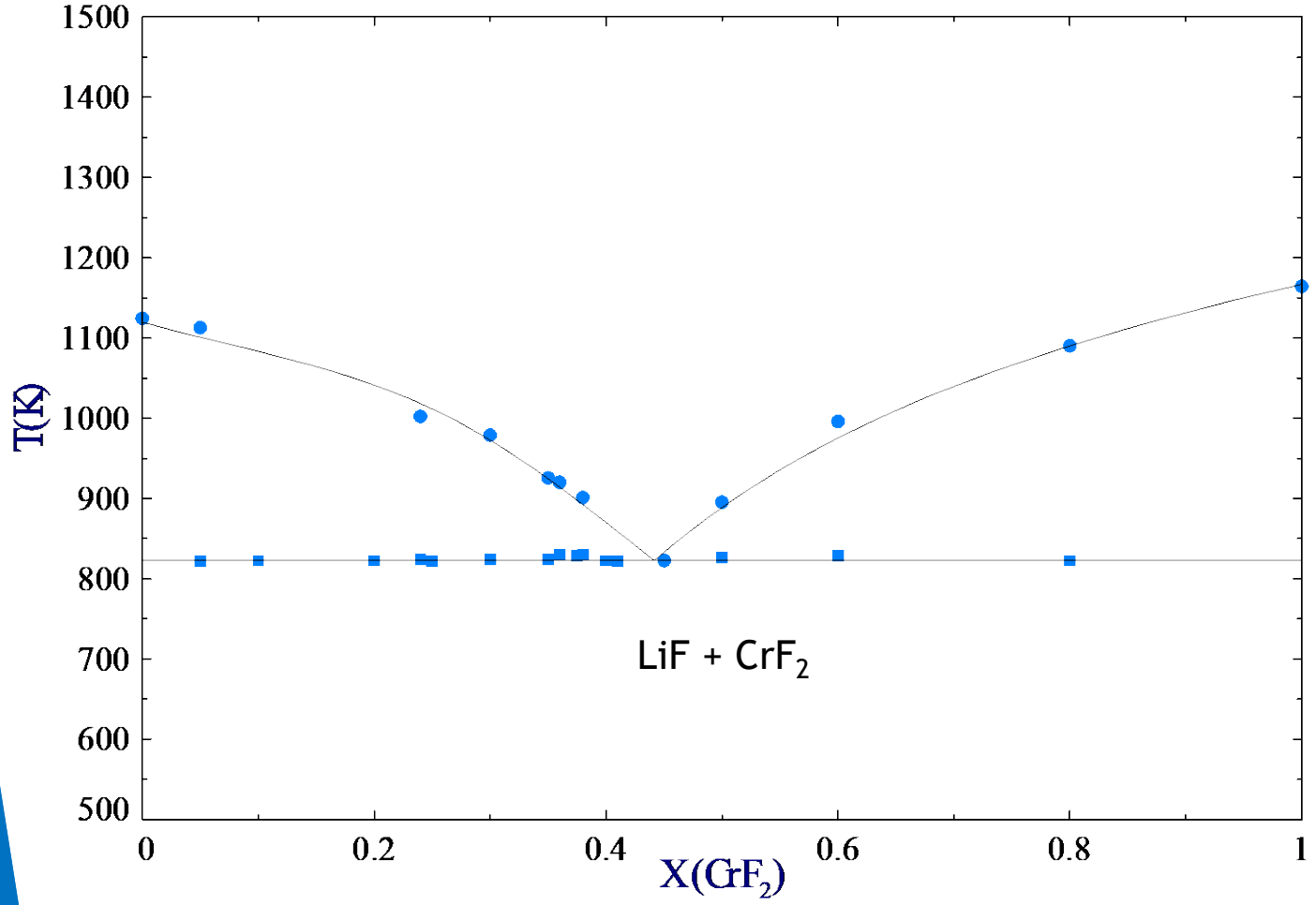


NH_4CrF_3 powder



CrF_2 powder

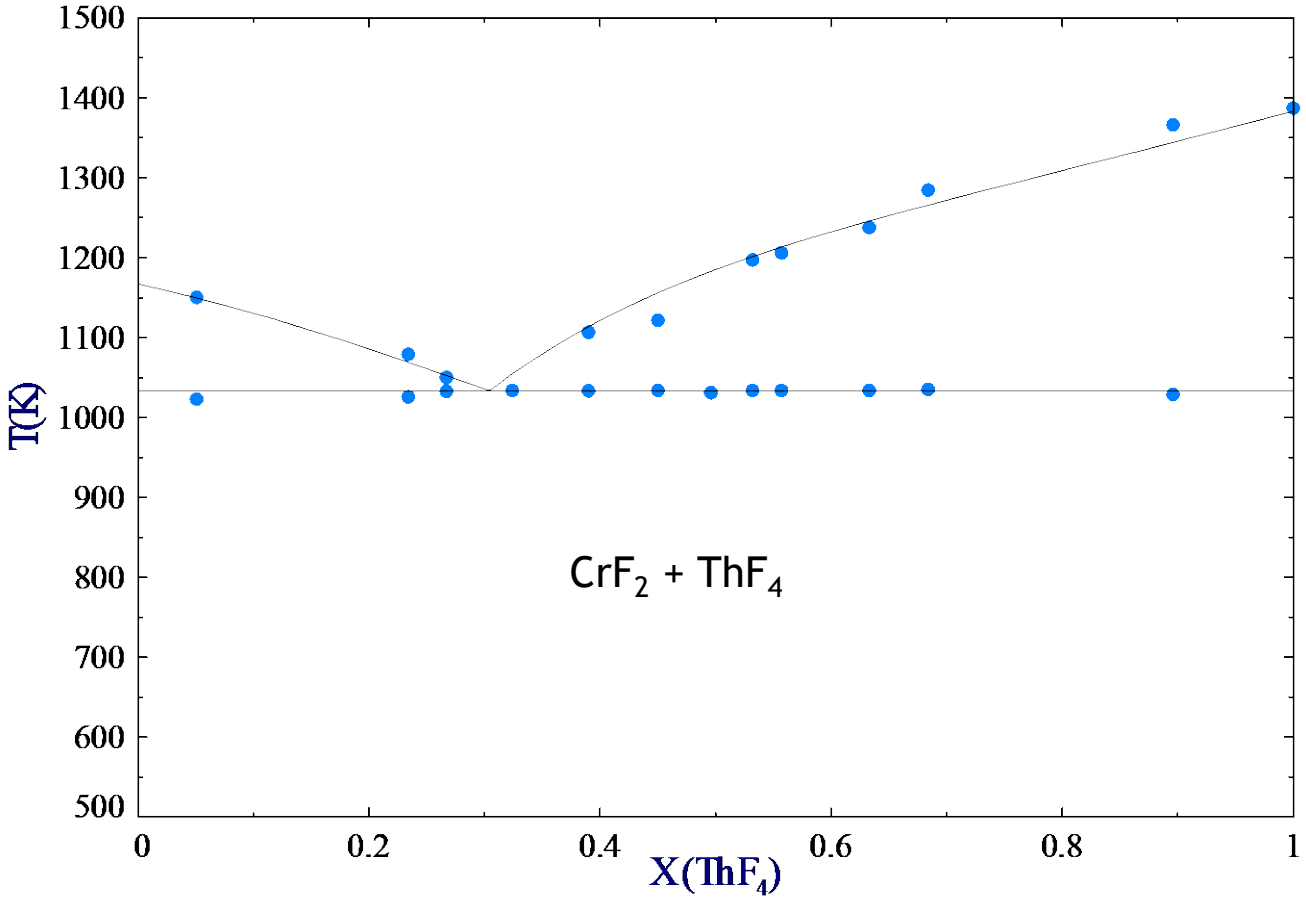
LiF-CrF_2 system



CALPHAD modeling of the LiF-CrF_2 system

- Optimization of the thermodynamic model based on collected phase diagram data by DSC and XRD

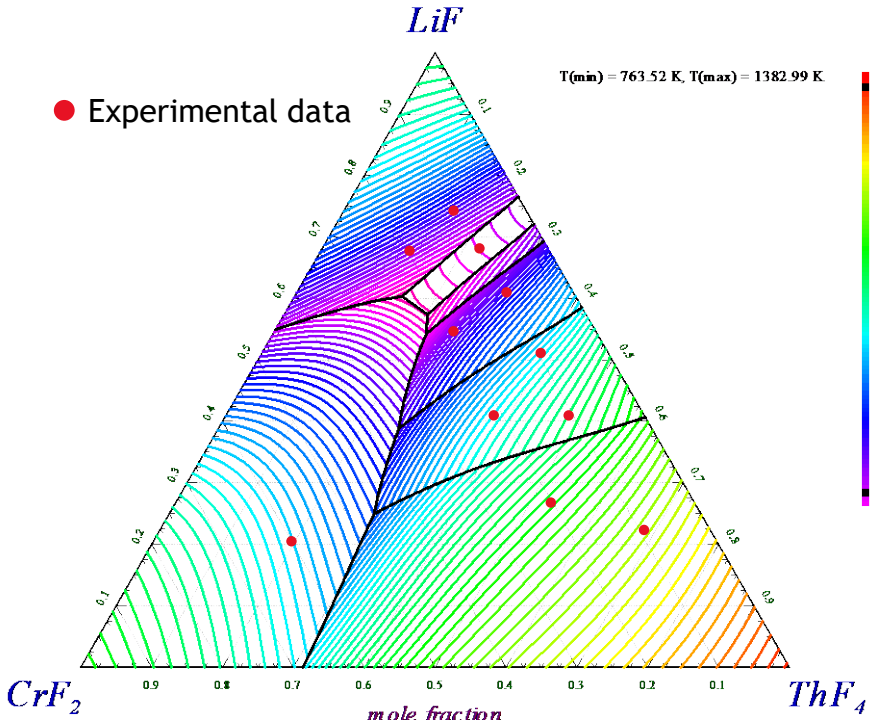
CrF_2-ThF_4 system



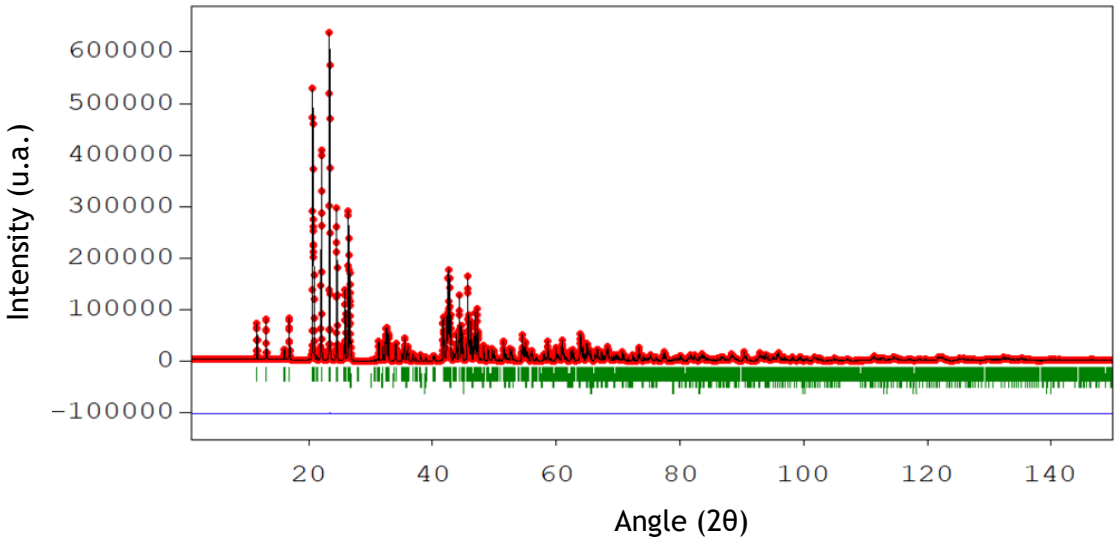
CALPHAD modeling of the CrF_2-ThF_4 system

- Optimization of the thermodynamic model based on collected phase diagram data by DSC and XRD

LiF-CrF_2-ThF_4 system



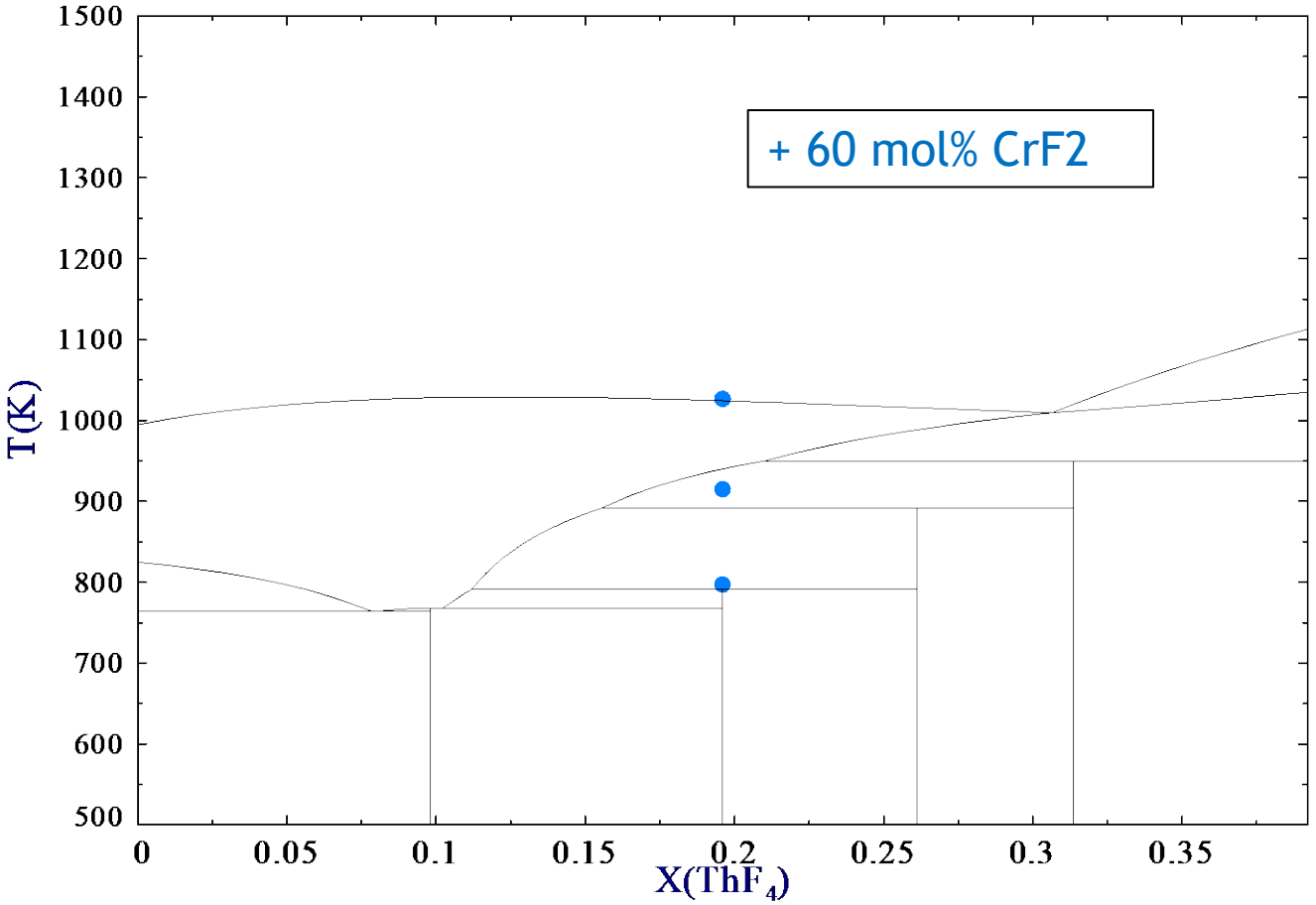
Liquidus projection of LiF-CrF_2-ThF_4

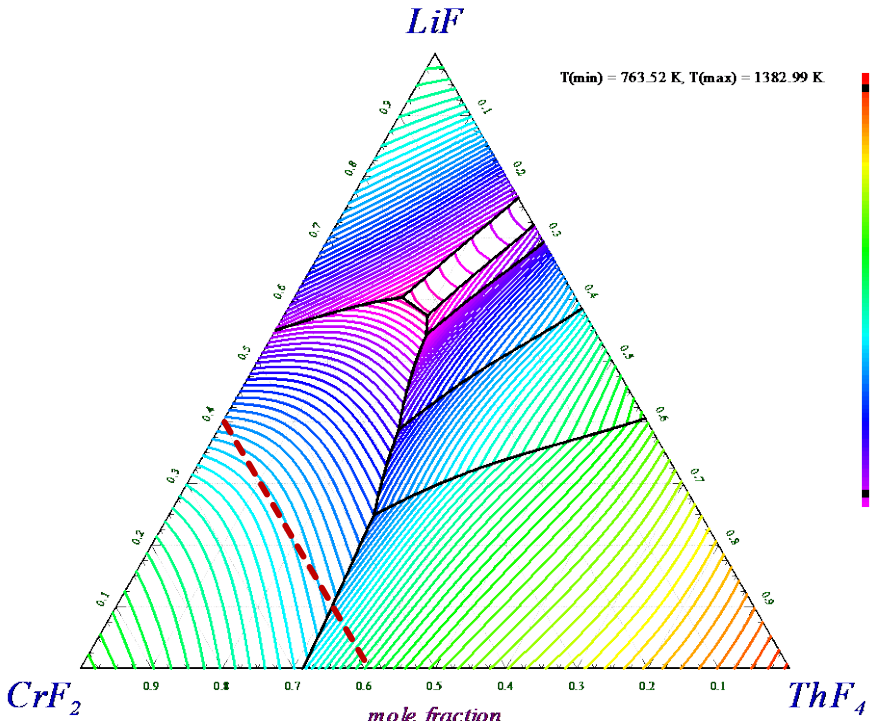


XRD pattern of the 0.2 LiF - 0.6 CrF_2 - 0.2 ThF_4 sample, no other compound than end-members are identified

$LiF\text{-}CrF_2\text{-}ThF_4$ system

- DSC measurement performed from X(ThF4) = 0.2 to 0.7 and optimization with the first data

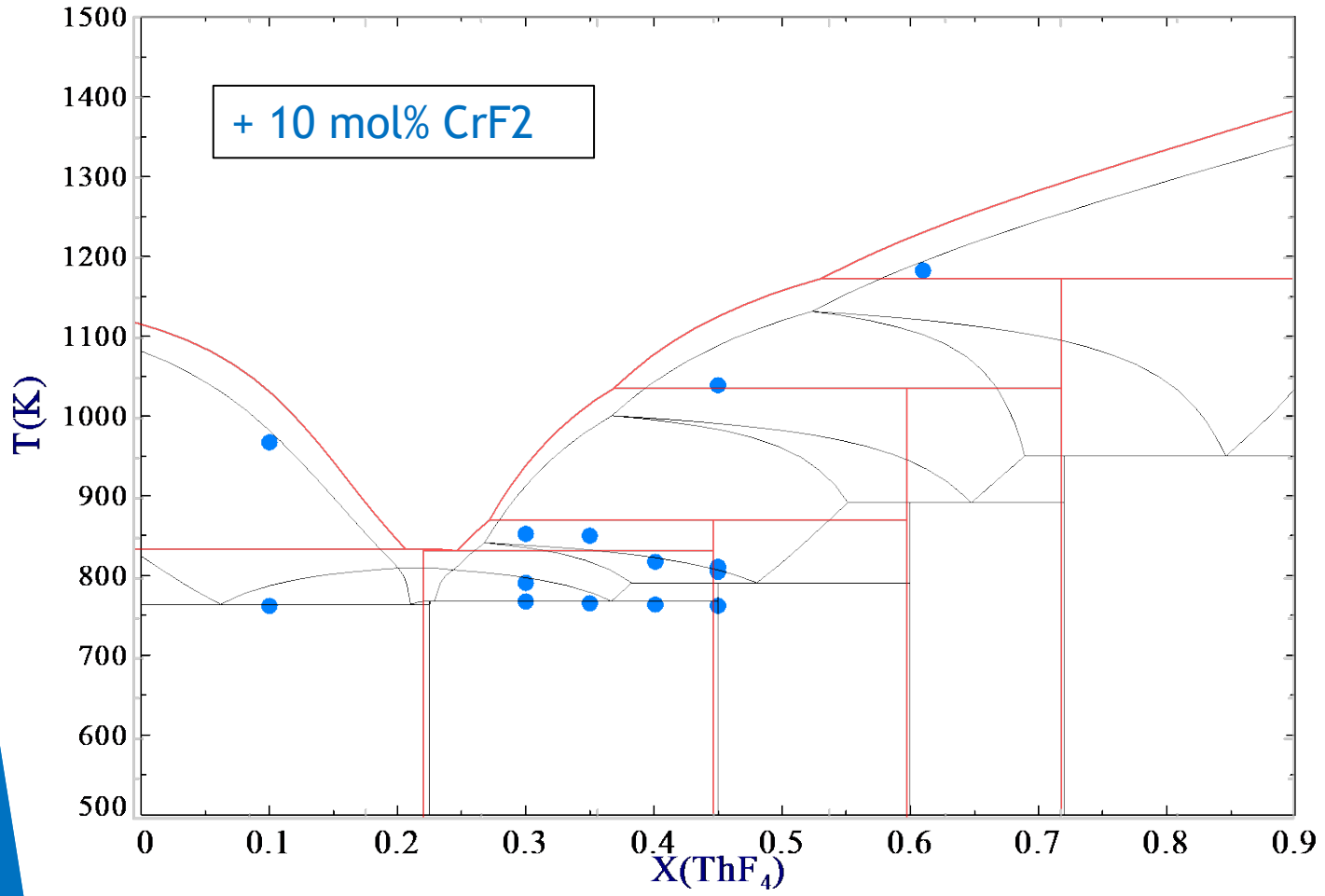


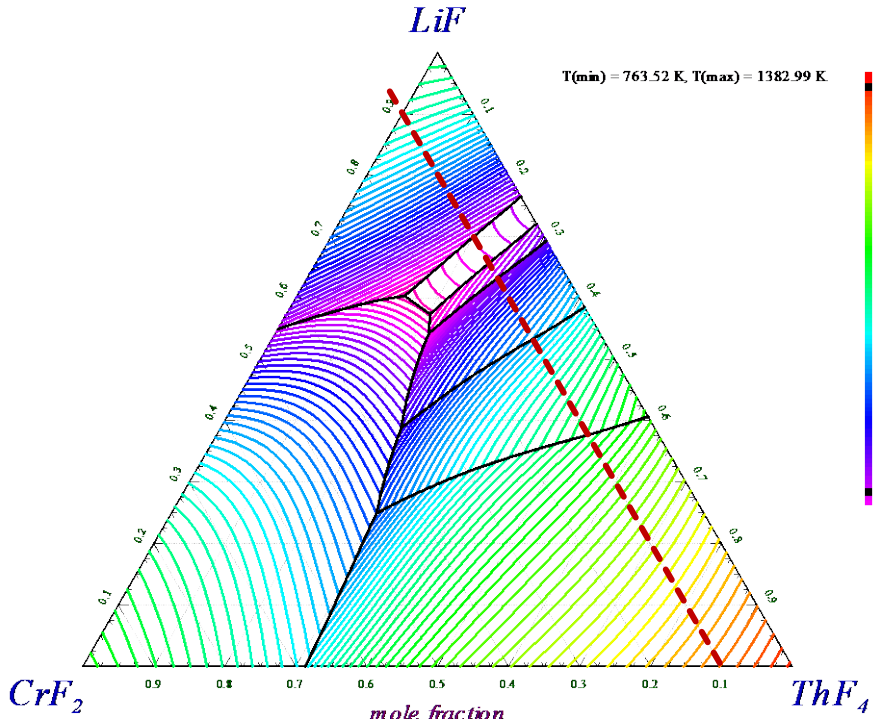


Pseudo-binary section on $LiF\text{-}CrF_2\text{-}ThF_4$ system at 60 mol% of CrF_2

$LiF\text{-}CrF_2\text{-}ThF_4$ system

- Data from the DSC measurements and fitting on the ternary phase diagram.





Pseudo binary on the composition 0.9 ($LiF\text{-}ThF_4$) + 0.1 CrF_2

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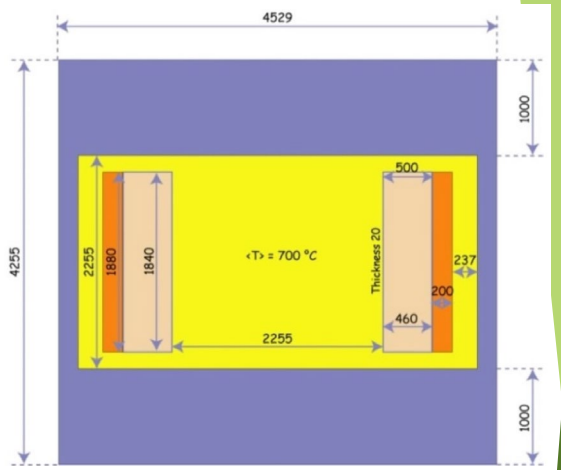
Impact of Fission products on Fuel behavior

Calculated composition of the fuel after 5 years operation:

Final fuel composition	
Nuclide(s)	**Mol (%)**
^{3}Li	71.94
^{90}Th	18.14
^{92}U	2.96
Total	**93.03**
Other compounds	
FPs 20<Z<73	**6.85**
Other	0.12

- Initial fuel: LiF - ThF_4 - UF_4 (77.5-19.5-3 mol%)
- Calculated in the framework of the SAMOSAFER project WP4 (PSI/TUD)
- Case study: no reprocessing

Major Fission Products (more than 0.045 mol %)			
Nuclide	**Z**	**Mol %**	**Chemical state(s)**
Zr	40	1.107	Fluoride – ZrF4
Xe	54	0.726	Noble gas
Mo	42	0.656	Metal
Nd	60	0.598	Fluoride – NdF3
Cs	55	0.594	Fluoride – CsF Iodide – CsI
Ce	58	0.469	Fluoride – CeF3
Sr	38	0.405	Fluoride – SrF2
Ru	44	0.259	Metal
Ba	56	0.253	Fluoride – BaF2
Y	39	0.211	Fluoride – YF3
La	57	0.209	Fluoride – LaF3
Kr	36	0.208	Noble gas
Pr	59	0.203	Fluoride – PrF3
Rb	37	0.189	Fluoride – RbF
Tc	43	0.140	Metal
Te	52	0.103	Metal
Sm	62	0.084	Fluoride – SmF3
I	53	0.065	Iodide – CsI
Rh	45	0.047	Metal
Pd	46	0.046	Metal
SUM		**6.573**	



Design: MSFR, Th fertile blanket, 3000 MW_{th}

Impact of Fission products on Fuel behavior

Fission products mixture in fluoride fuel:

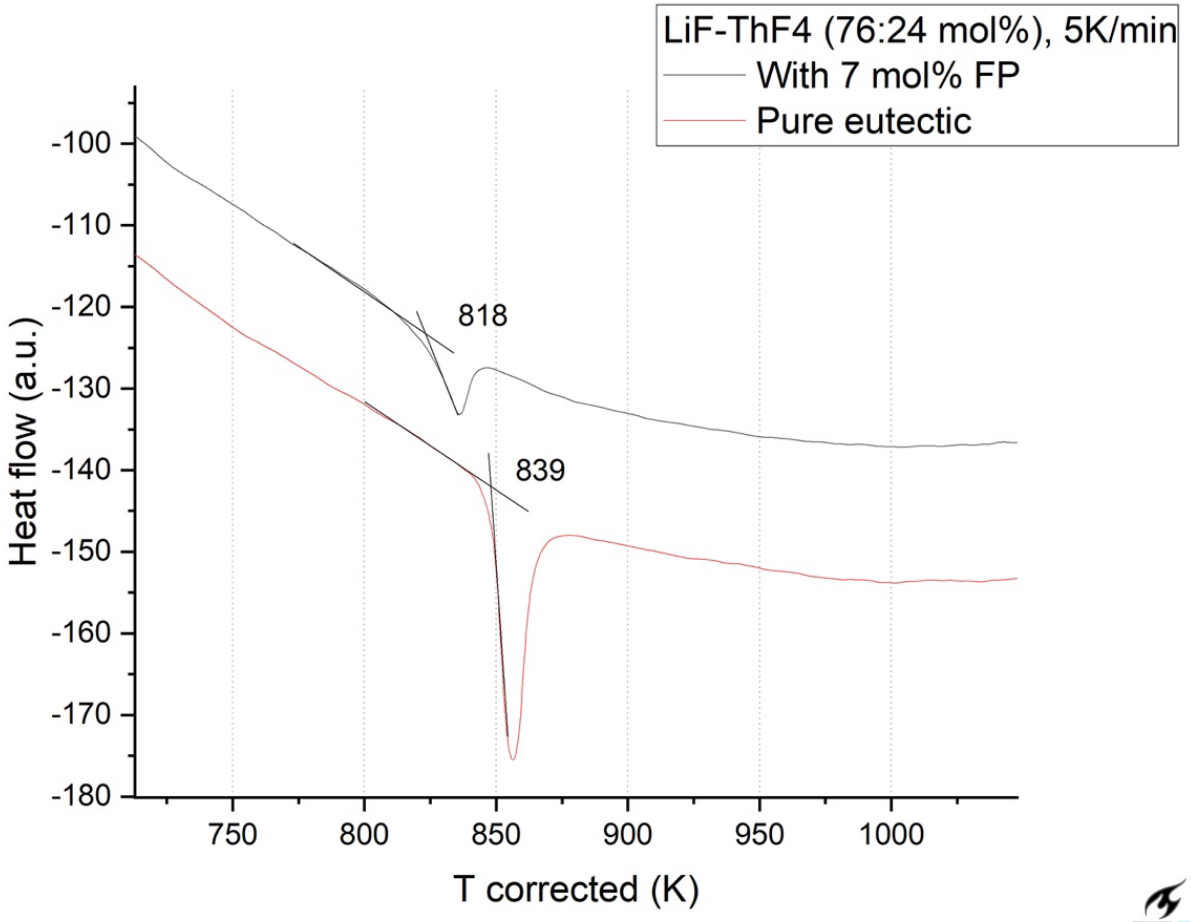
End-members	Mol %	Melting temperature
ZrF4	25.2	910 °C/1183 K
NdF3(La,Pr,Sm)	24.9	1374 °C/1647 K
CsF	12.1	703 °C/976 K
CsI	3.0	621 °C/894 K
CeF3	10.7	1460 °C/1730 K
SrF2(Ba)	15.0	1477 °C/1750 K
YF3	4.8	1387 °C/1660 K
RbF	4.3	785 °C/1068 K

- Fuels:
  - $LiF - ThF_4$ (76 - 24 mol%)
  - $LiF - ThF_4 - UF_4$ (77.5 - 19.5 - 3 mol%)
  - $NaF - KF - UF_4$ (50.4 - 23.2 - 26.4 mol%)
- Mixture of fuel + 7 mol% FPs (maximal accumulation of fission products)

Impact of Fission products on Fuel behavior

Impact of fission products on the fuel salt melting temperature measured by DSC:

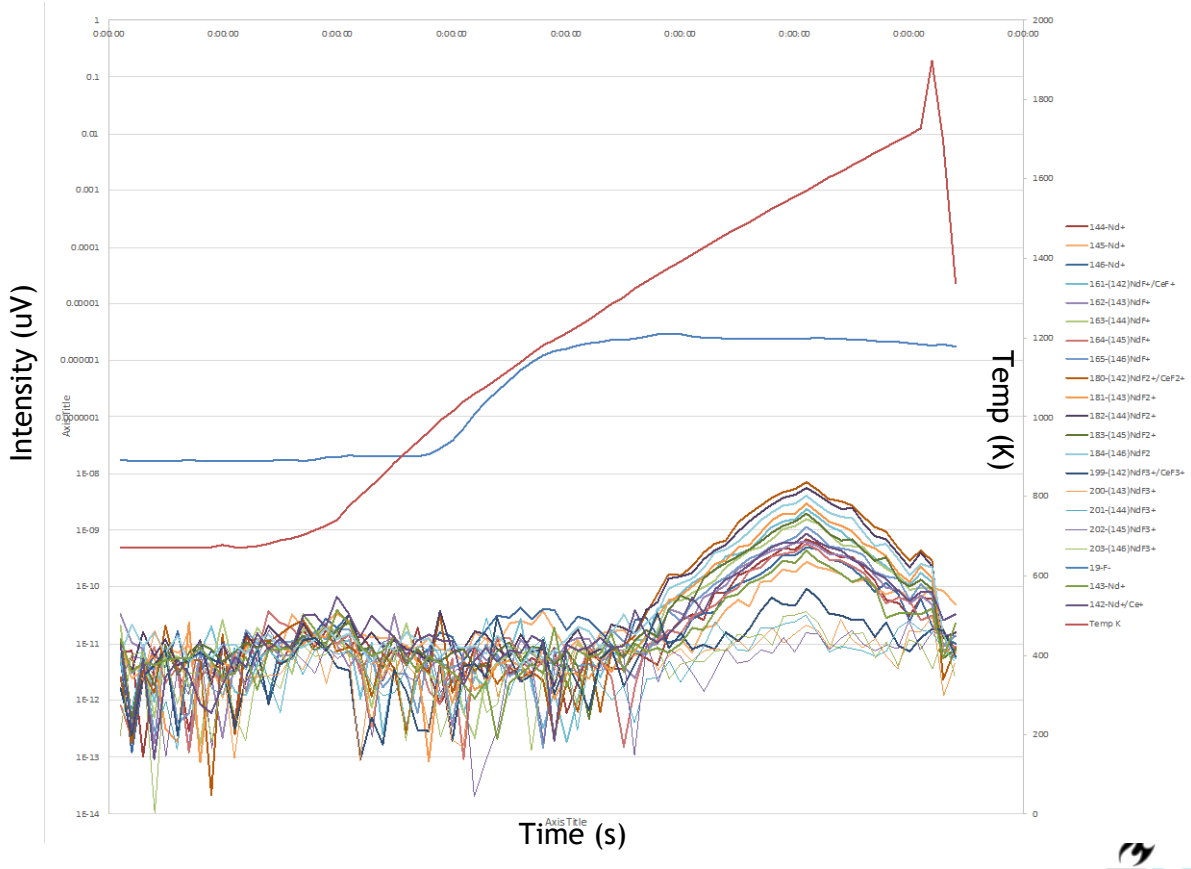
- Very low impact on the thermodynamic properties



Impact of Fission products on Fuel behavior

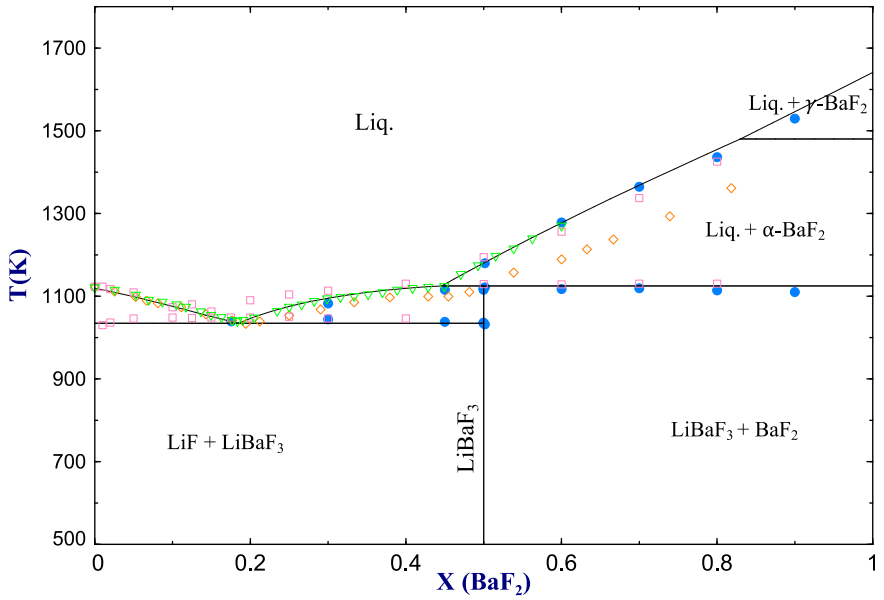
Impact of fission products on the fuel salt vapor pressure measured by KEMS

- Total vaporization behavior of the fuels is not affected by the presence of fission products
- Overall solubility of the fission products except CsI

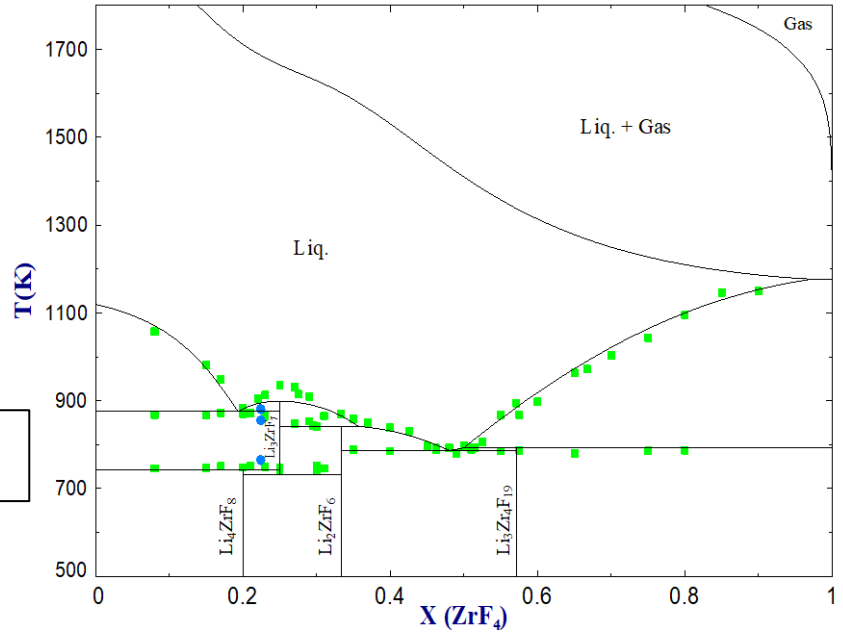


KEMS analysis of the different neodymium species

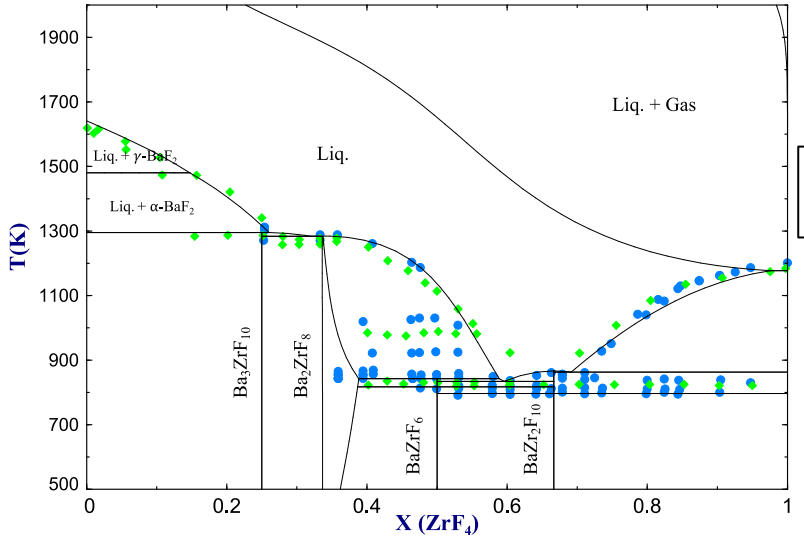
$LiF\text{-}BaF_2$, $LiF\text{-}ZrF_4$ and $BaF_2\text{-}ZrF_4$ systems modeling



Phase diagrams of the binary system $LiF\text{-}BaF_2$



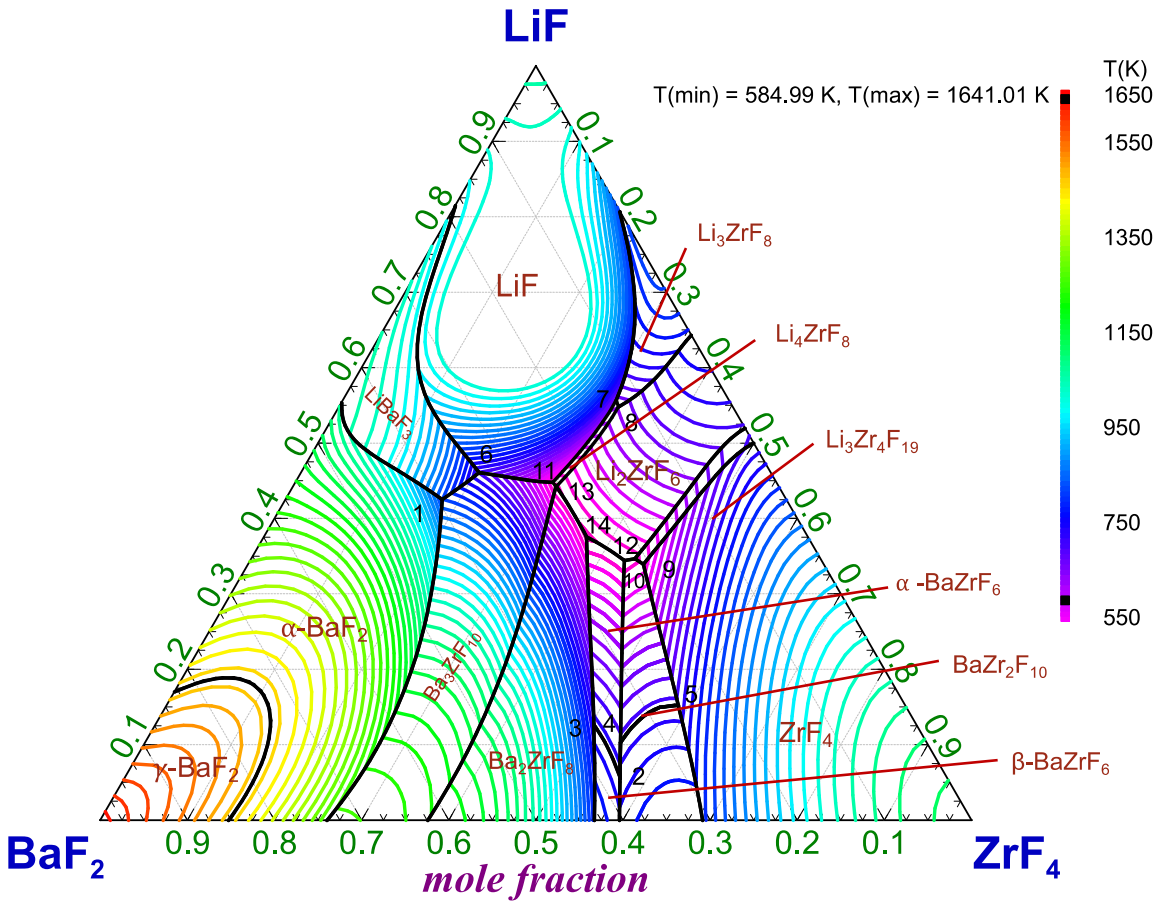
Phase diagrams of the binary system $LiF\text{-}ZrF_4$



Phase diagrams of the binary system $BaF_2\text{-}ZrF_4$

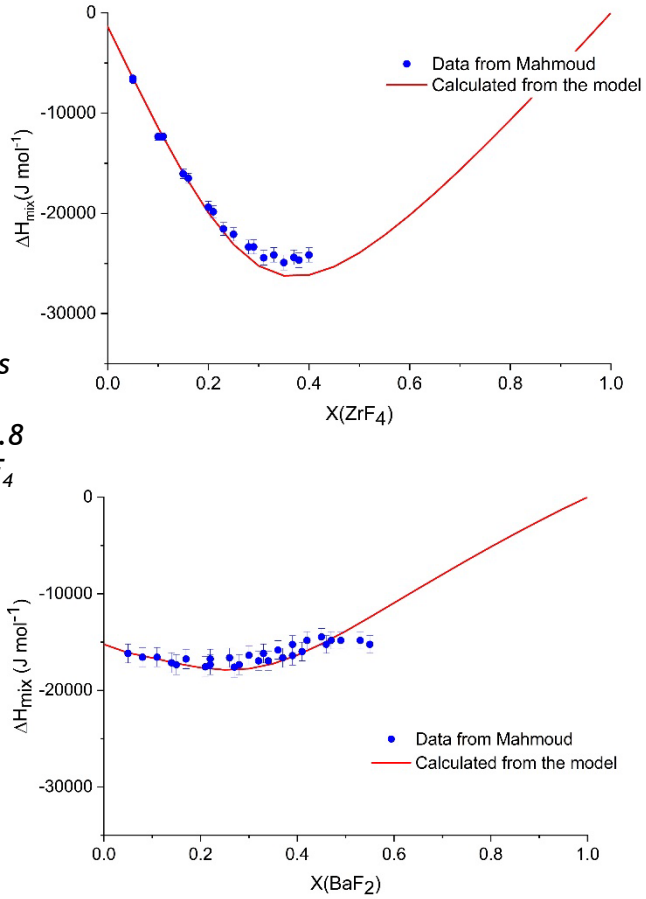
- On-going publication

LiF-BaF_2-ZrF_4 systems modeling



Liquidus projection of the ternary system LiF-BaF_2-ZrF_4, optimized in this work

Mixing enthalpies of the pseudo-binary sections (0.8 LiF+0.2 BaF_2)-ZrF_4 and (0.8 LiF+0.2 ZrF_4)-BaF_2



- On-going publication

Acknowledgement

T. Dumaire acknowledges gratefully financial support from the Nuclear Research and Consultancy Group (NRG, Petten, Netherlands) and the SAMOSAFER project which has received funding from the Euratom research and training program 2014-2018 under grant agreement N°847527. Many thanks to the SAMOSAFER project's mobility scheme for its help during the secondment to the JRC-Karlsruhe.

Application of multiphysics calculations on 5M particle simulation

Stefano Lorenzi (PoliMi)

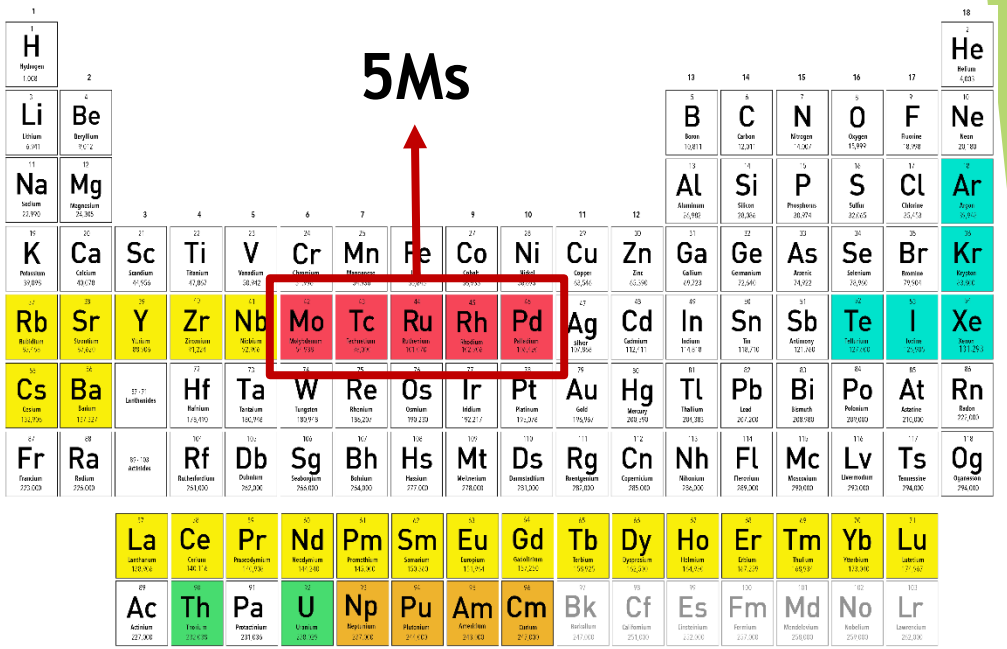
SAMOSAFER Final Meeting

28 November 2023, Avignon, France

The Noble Metals Issue

- **Very low solubility** in the salt → behave as **particles** transported by the flow
- Close together on the periodic table → grouped approach in the following
- **Deposition** on surfaces → Deterioration of heat transfer; Decay hot spots
- Bubbling system for **removal** is foreseen

Need for a Multiphysics modeling approach!



Overview of the key elements expected in the salt during normal operations. In green the fuel species, in orange the TRUs, in yellow the soluble FPs, in blue the GFPs and **in red the 5Ms**.

Modelling approach

Transport equations for solid FP

Single-phase Eulerian advection-diffusion-decay equation

$$\frac{\partial c_i}{\partial t} = \nabla \cdot \left(D_{eff} \nabla c_i\right) - \nabla \cdot \left(c_i \boldsymbol{u}\right) - \lambda_i c + S_i$$

DECAY CONSTANT

FP VOLUMETRIC CONCENTRATION (at m^{-3})

Concentration-driven turbulent dispersion

$$D_{eff} = D + D_t = \frac{\nu}{Sc} + \frac{\nu_t}{Sc_t}$$

TURB. SCHMIDT NUMBER

Modelling and numerical treatment of deposition

Particle deposition on the wall

$$\frac{\partial d}{\partial t} = -\lambda d - \xi d + \gamma C$$

DEPOSITION RATE

Mixed-type boundary (wall) conditions

$$-D_{eff} \nabla c_i \cdot \boldsymbol{n} = \gamma c_i$$

FP SURFACE DEPOSITION FLUX (at $m^{-2}\ s^{-1}$)

DEPOSITION VELOCITY

Temperature effects on precipitation-dissolution of particles

Simplified precipitation-dissolution reaction for a metal species

$$M + nUF_4 \rightleftarrows MF_n + nUF_3$$

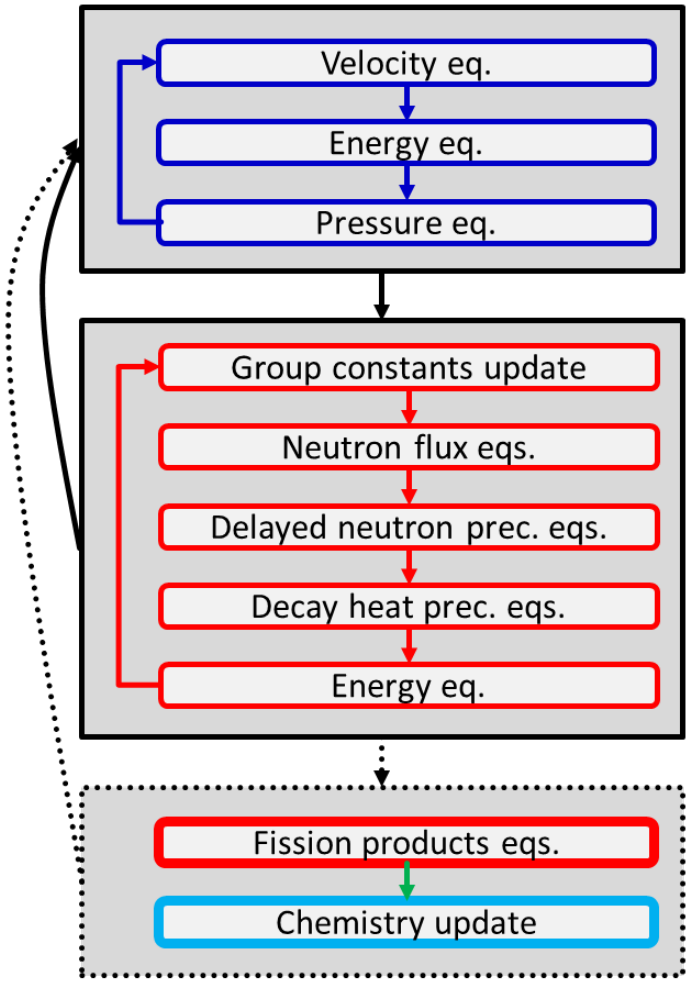
$$[M^{n+}] \cong K(T) \left(\frac{[U^{4+}]}{[U^{3+}]}\right)^n$$

EQ. CONSTANT

UF_4/UF_3 RATIO (constant ≈ 100)

Van 't Hoff equation

$$\log \frac{K(T_2)}{K(T_1)} = \frac{\Delta H^\circ}{R} \left(\frac{1}{T_1} - \frac{1}{T_2}\right)$$



Modelling approach

Simulation of 5M scenario

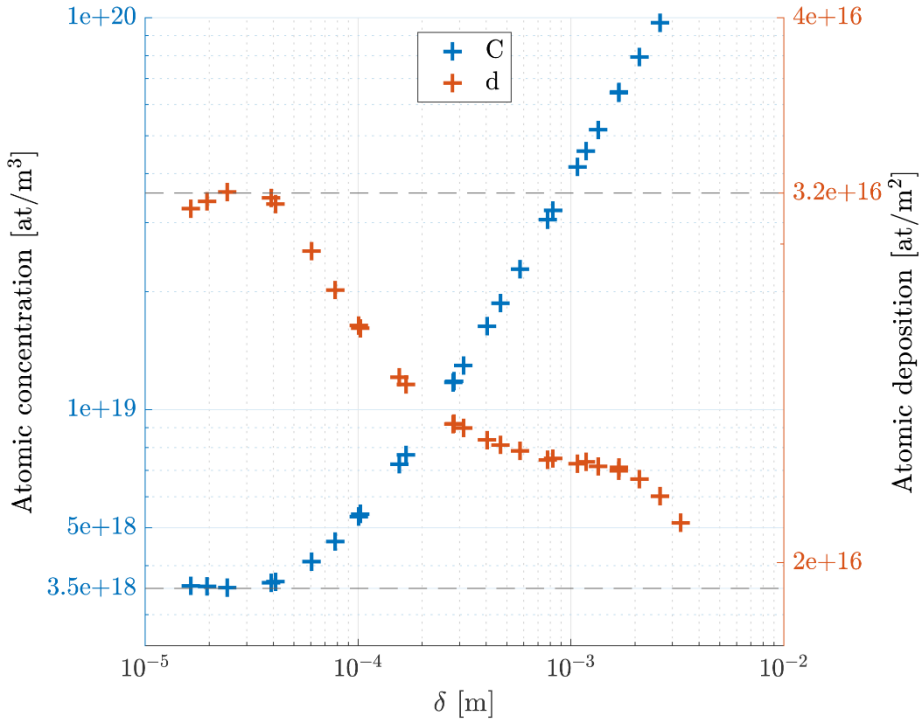
- **Aim**: Simulation of the transport of solid FPs constituted by “noble metal” species (Mo, Rh, Ru, Pd, Tc). This should include deposition on the wall and possible precipitation-dissolution effects to the temperature transients.
- **Modelling assumptions:**
  - Chemical equilibrium constant for Van’t Hoff eq
  - Deposition on the wall with dep. velocity BC
  - 5M clustering to minimize the computational effort

Deposition on the wall

Deposition on the wall → “Perfect sink” wall condition

$$C_i\Big|_{\partial\Omega} = 0$$

Mesh refinement down to approx. 10^{-3} m or less is needed close to walls to resolve the concentration boundary layer



Velocity deposition wall condition

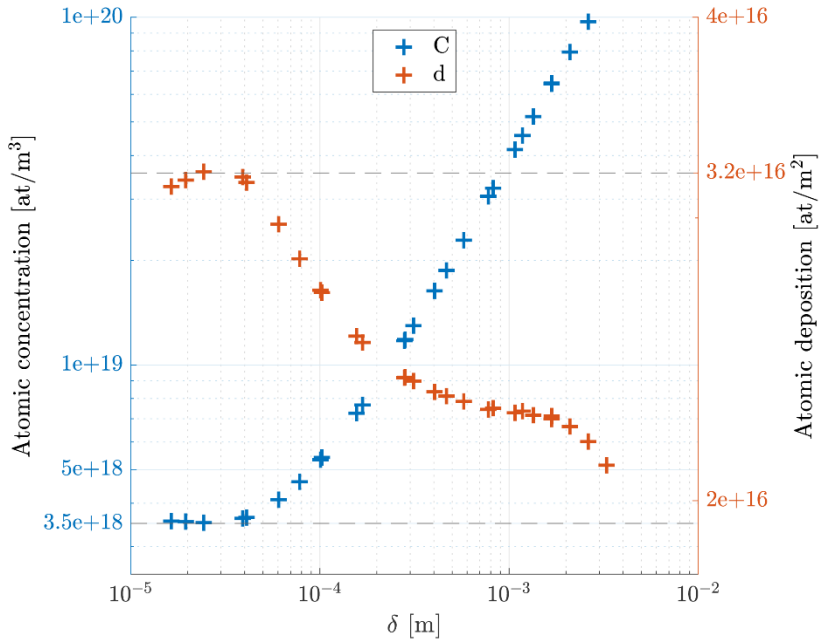
$$-D_{eff}\nabla c_i \cdot \boldsymbol{n} = \gamma c_i$$

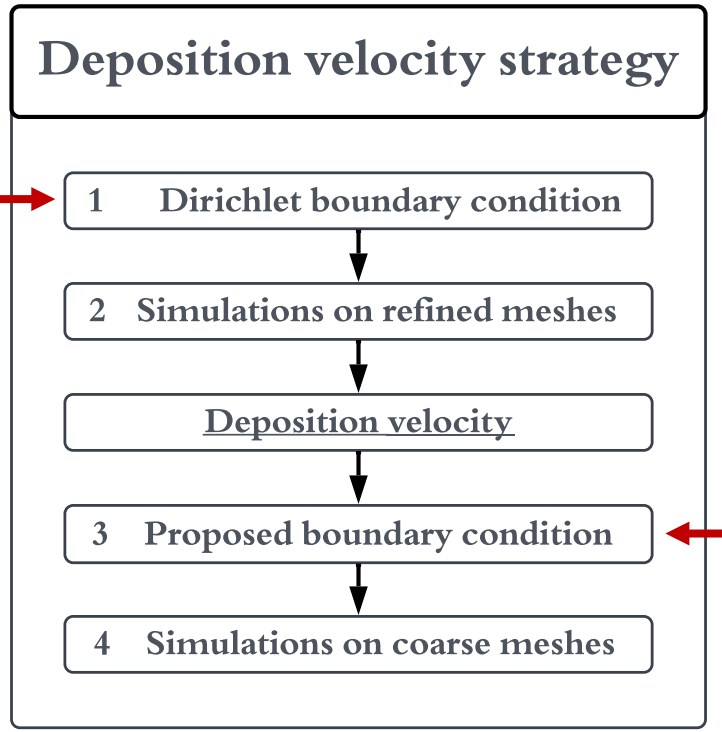
γ is the velocity deposition (mm/s)

Deposition on the wall - BCs

Null Dirichlet BC

$C = 0 \quad @\, walls$





Deposition velocity BC

$-D_{eff} \nabla C \cdot \vec{n} = \boldsymbol{\gamma} C$

Mixed BC (Robin) in OpenFOAM

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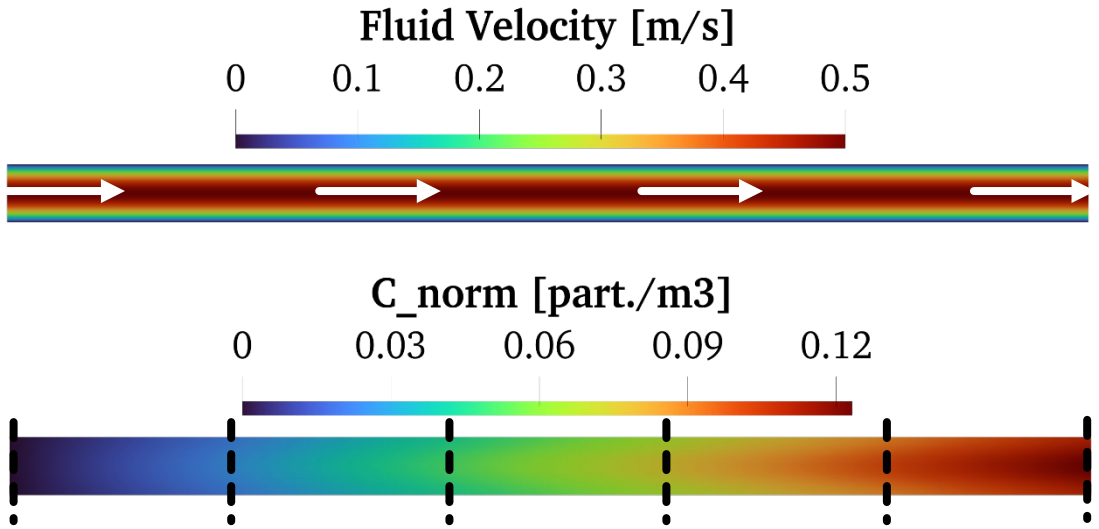
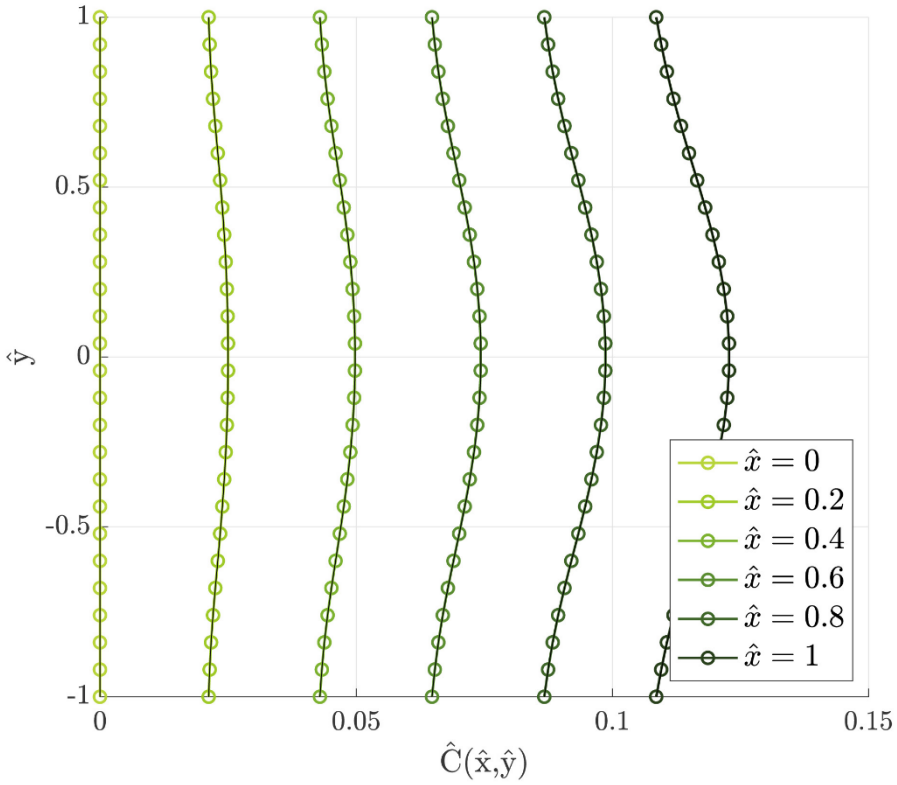
Deposition on the wall - Verification

Available Analytical Solution

2D Laminar flow between parallel plates



Results using the proposed OpenFOAM model.



Comparison of normalized concentration profiles at different normalized lengths $\hat{x}$, obtained with the proposed OpenFoam model (◦) and the analytical solution (−).

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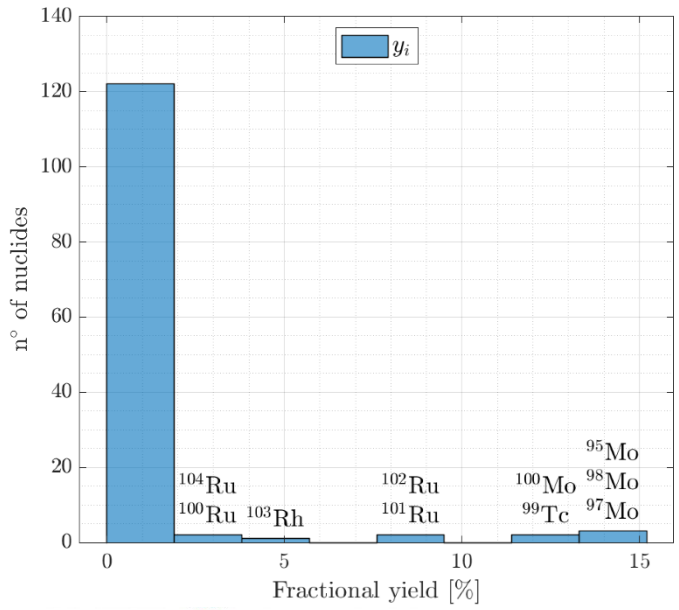
5M simulation: clustering

Clustering of the 5M according to their property to minimize the computational effort

- 5Ms are chemically and physically very similar
- Nuclear species show a broad range of λ, but the prevalent ones are rather slow-decaying
- One pseudo-nuclide to be considered as initial step

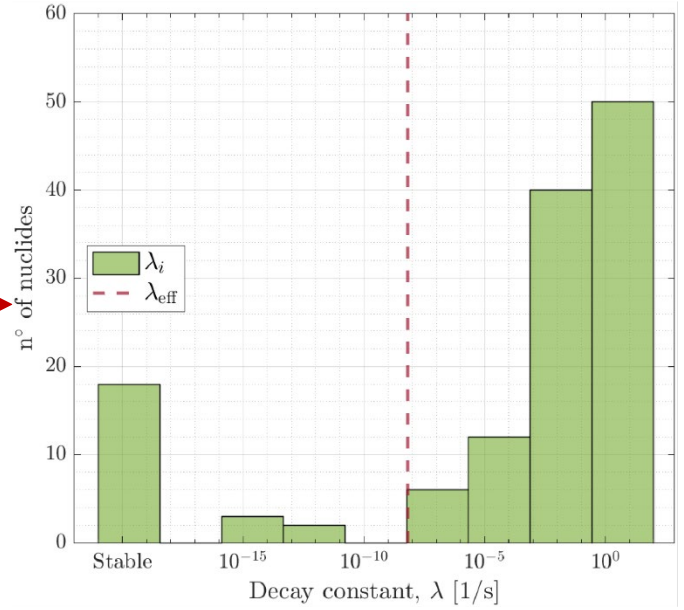
$$\frac{\partial C}{\partial t} + \nabla \cdot (\boldsymbol{u}C) = \nabla \cdot \left(\boldsymbol{D_{eff}} \nabla C\right) - \boldsymbol{\lambda_{eff}} C + \boldsymbol{y_{tot}} R_f$$

ρ (kg/m³)	d_p (m)	y_{tot} (-)	λ_{eff} (1/s)
$1.098 \cdot 10^4$	$370.3 \cdot 10^{-12}$	0.295	$6.614 \cdot 10^{-9}$

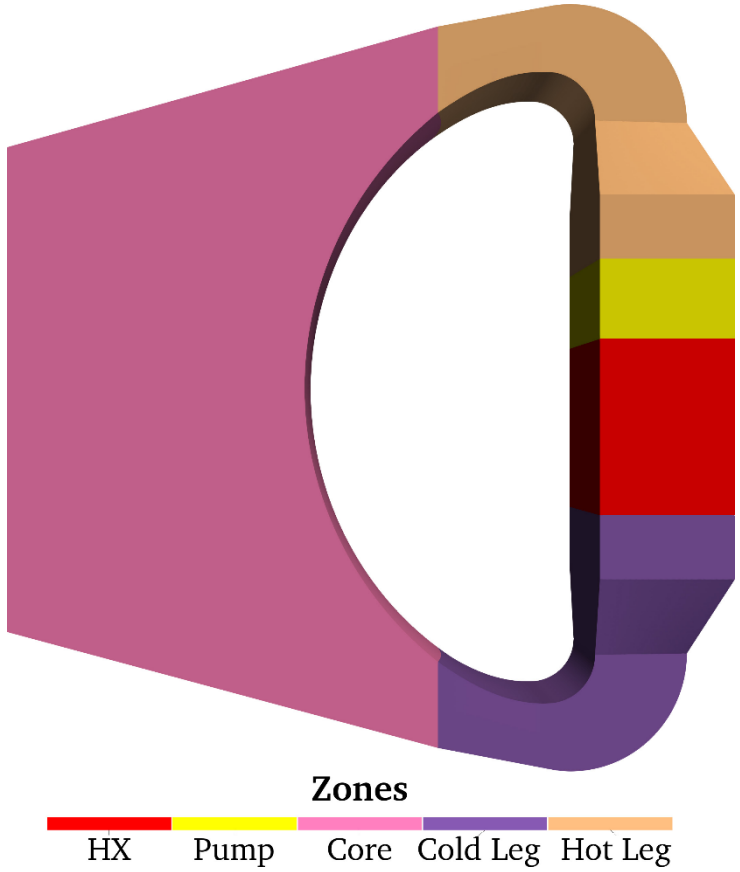


Homogeneous radioactive mixture hypothesis

$$A_{mix} = \sum_{i=1}^{n} \lambda_i y_i = \lambda_{eff} y_{tot}$$



5M simulation



Simplified reactor zones in the employed geometry.

Case	n° cells	Bulk cell size (mm)	Wall cell size (mm)	Total wall faces
1	85’560	30	-	13034
2	159’624	30	5.0	13034
3	209’960	30	2.5	13034
4	543’244	20	1.0	28160
5	595’812	20	0.5	28160
6	4’345’352	9	0.3	133116

Key properties of the six meshes used for the investigation

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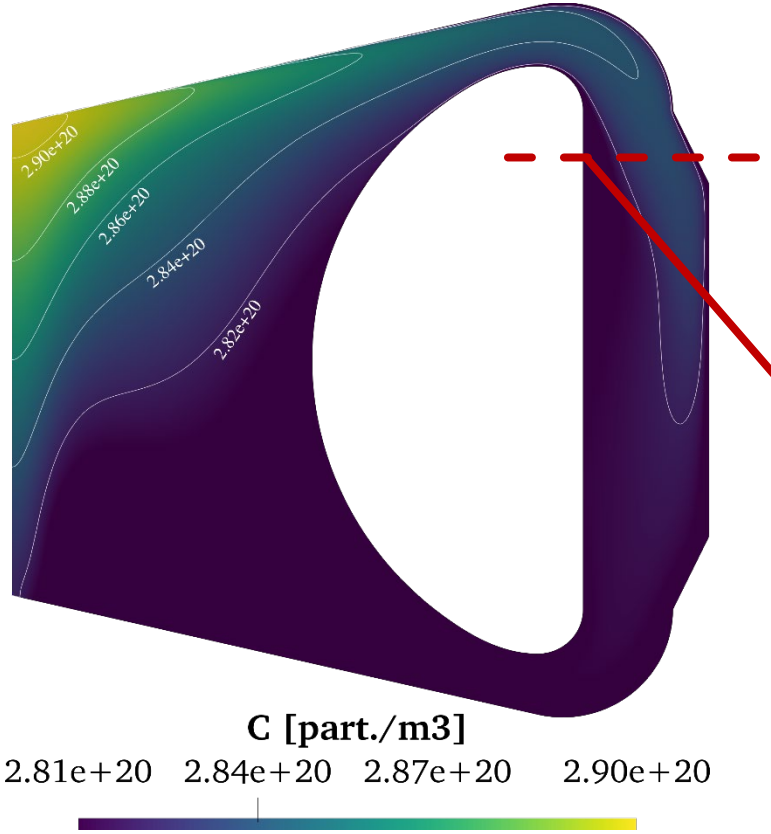
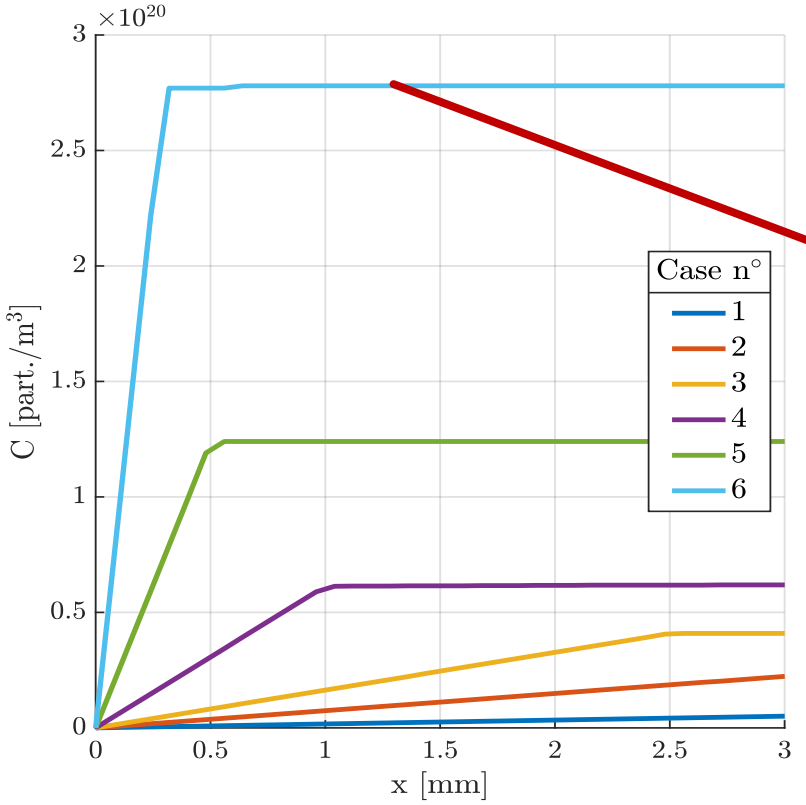
5M simulation: FP concentration with null Dirichlet BC



5Ms particle distribution shown across an axisymmetric slice, mesh case 6.



5Ms particle concentration profiles close to the left wall along an arbitrary line.

1 Dirichlet boundary condition

2 Simulations on refined meshes

Deposition velocity

$$\gamma = \frac{-D_{eff}\nabla C \cdot \vec{n}}{C_{avg}}$$

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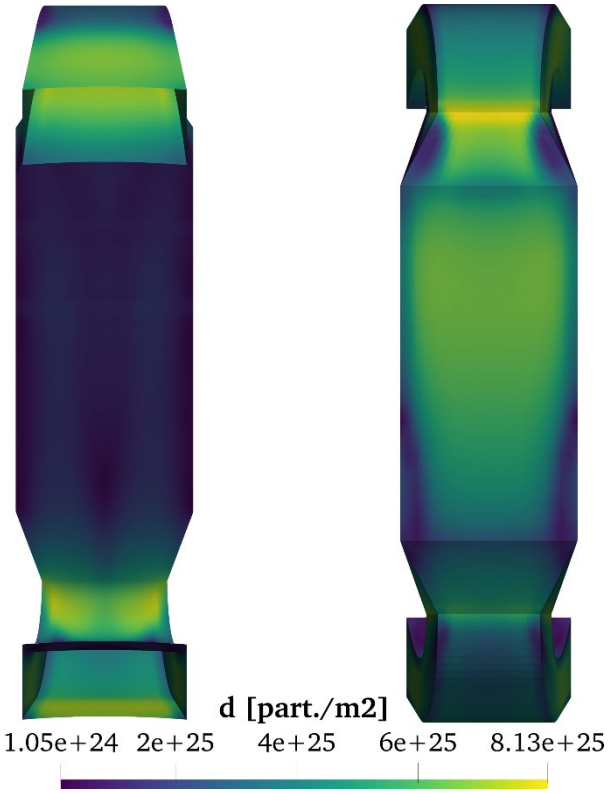
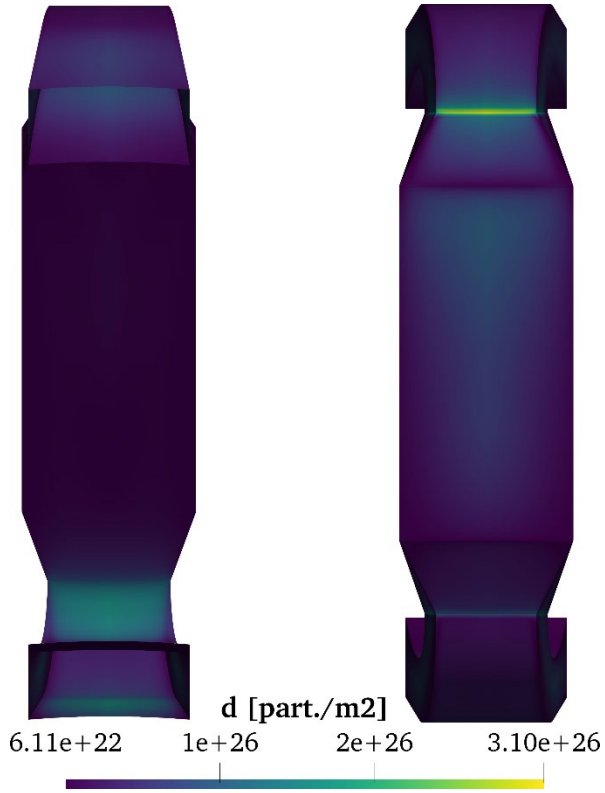
5M simulation: FP deposition with null Dirichlet BC



5Ms particle deposition at steady state on the outer loop, inside and outside view of case 1.



5Ms particle deposition at steady state on the outer loop, inside and outside view of case 6.

Case	Tot deposited particles	d (part./m^2)
1	2.530×10^{26}	1.07×10^{25}
2	2.533×10^{26}	5.23×10^{24}
3	2.530×10^{26}	9.62×10^{24}
4	2.532×10^{26}	1.28×10^{25}
5	2.531×10^{26}	6.60×10^{24}
6	2.452×10^{26}	4.00×10^{24}

5Ms particle deposition key quantities for all the six mesh cases. “d” values are sampled at the wall on the same line previously highlighted.

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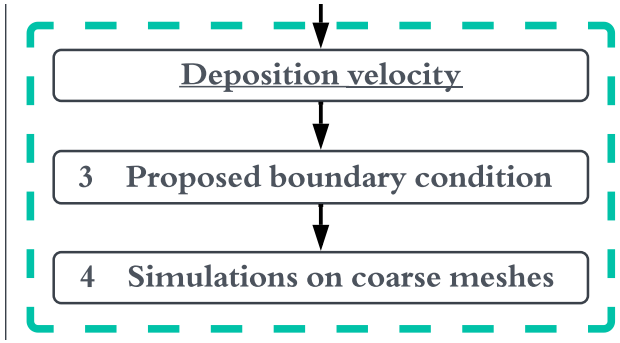
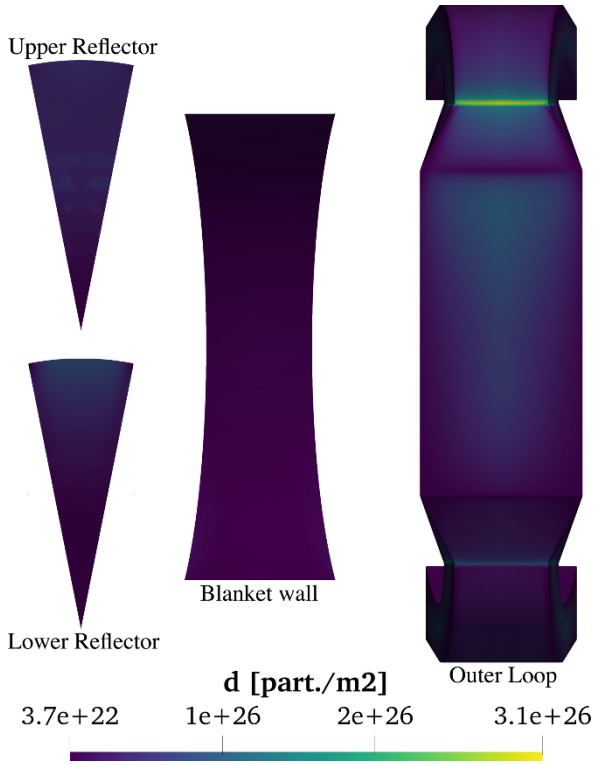
5M simulation: FP concentration with velocity deposition BC

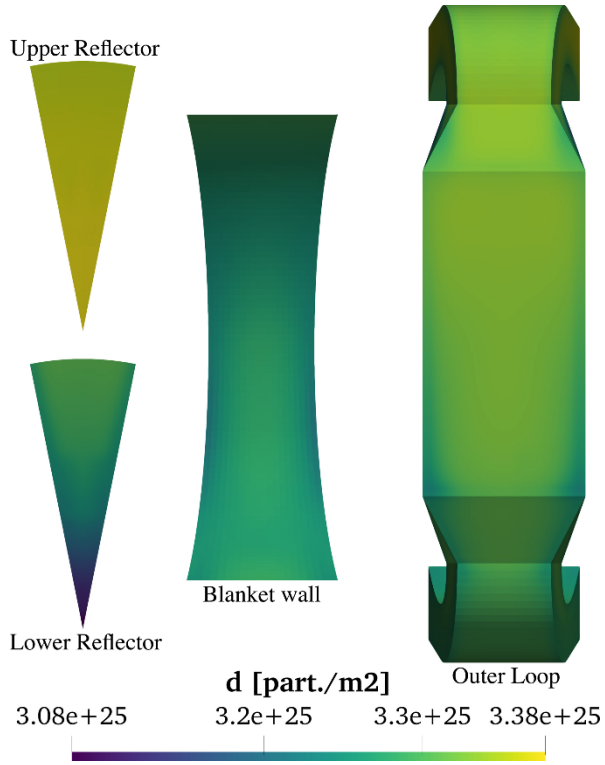


$$-D_{eff}\nabla C \cdot \vec{n} = \gamma C$$

Mixed BC (Robin) in OpenFOAM



Reference case, mesh **6.**
CPU*h: 1500

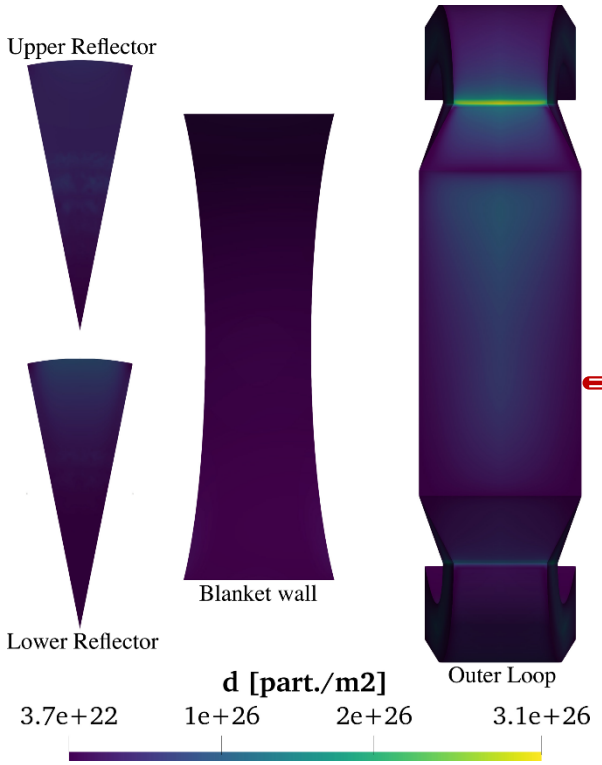


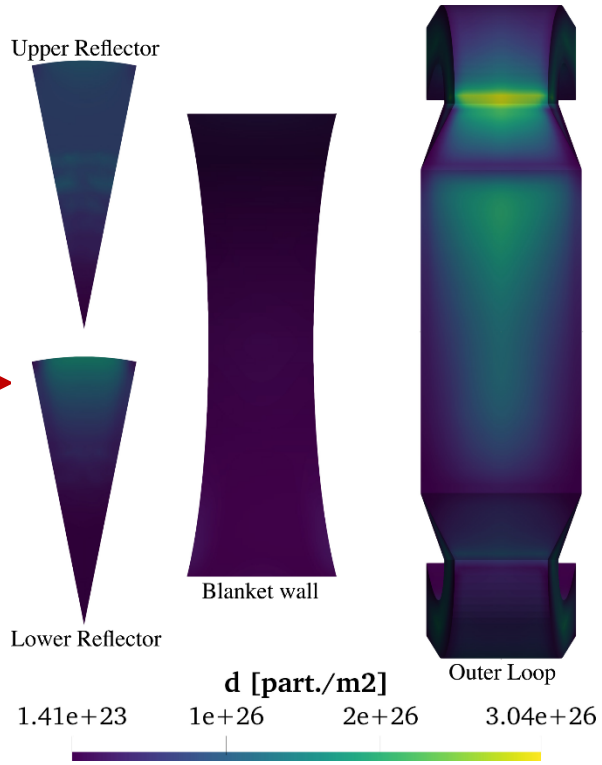
Proposed **BC**, mesh 2.
CPU*h: 45

What's wrong?

5M simulation: FP concentration with velocity deposition BC

What's wrong? γ is not uniform inside the reactor. Make it a field!





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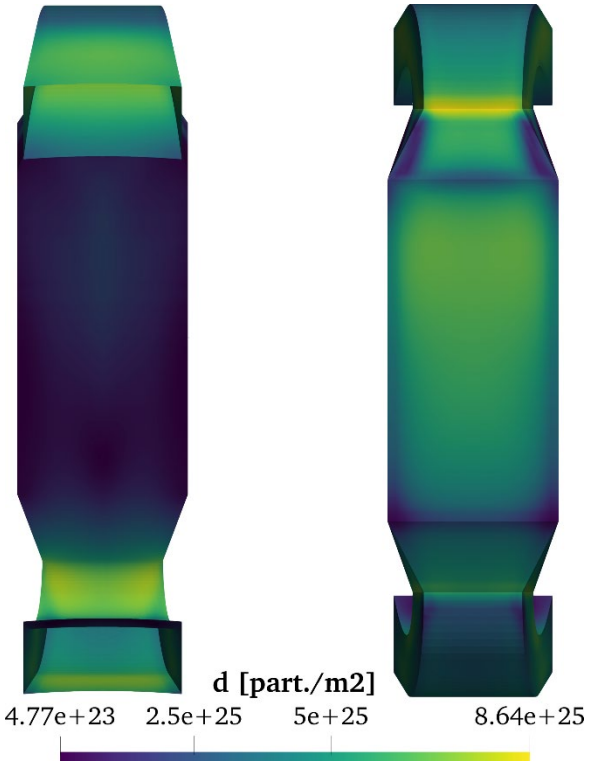

Reference case, mesh **6.**
CPU*h: 1500

Proposed BC, mesh **2.**
CPU*h: 45

Null Dirichlet, mesh **2.**
CPU*h: 45

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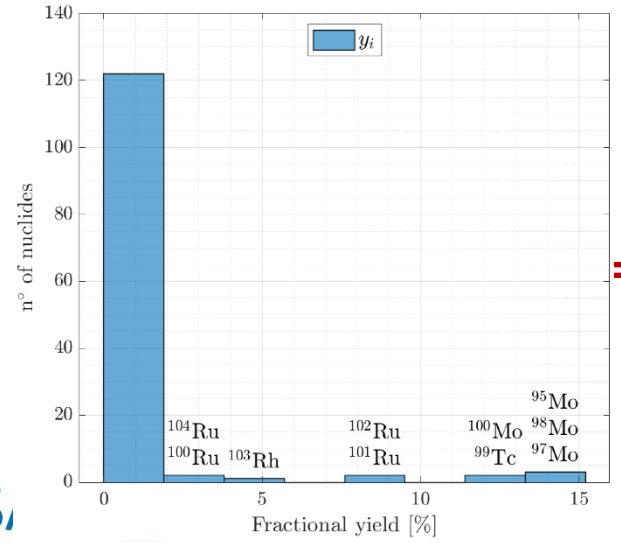
5M simulation

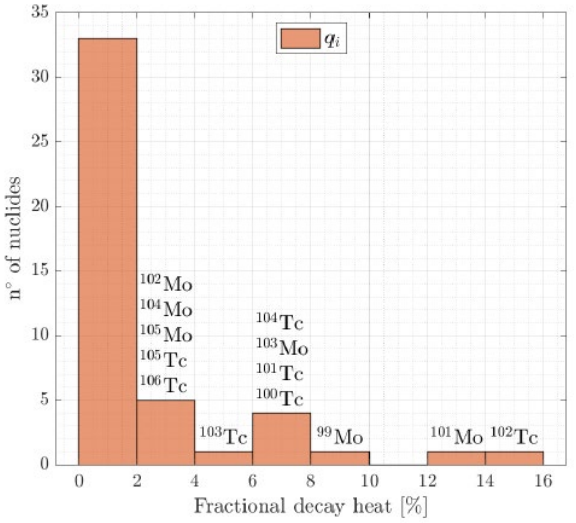
What about decay heat?

- Heat from a decay event within the deposited layer accumulating on the Fuel Circuit
- Similar approach of the 5M clustering
- 5M are not the main contributors, we should include also metal particles (but some of them could be dissolved in the salt)

	ρ (kg/m³)	d_p (m)	y_{tot} (-)	λ_{eff} (1/s)	Q_{eff} (W/part)
5M	$1.098 \cdot 10^4$	$370.3 \cdot 10^{-12}$	0.295	$6.614 \cdot 10^{-9}$	$2.146 \cdot 10^{-21}$
Metals	$6.786 \cdot 10^4$	$436.6 \cdot 10^{-12}$	1.248	$2.336 \cdot 10^{-8}$	$9.335 \cdot 10^{-21}$

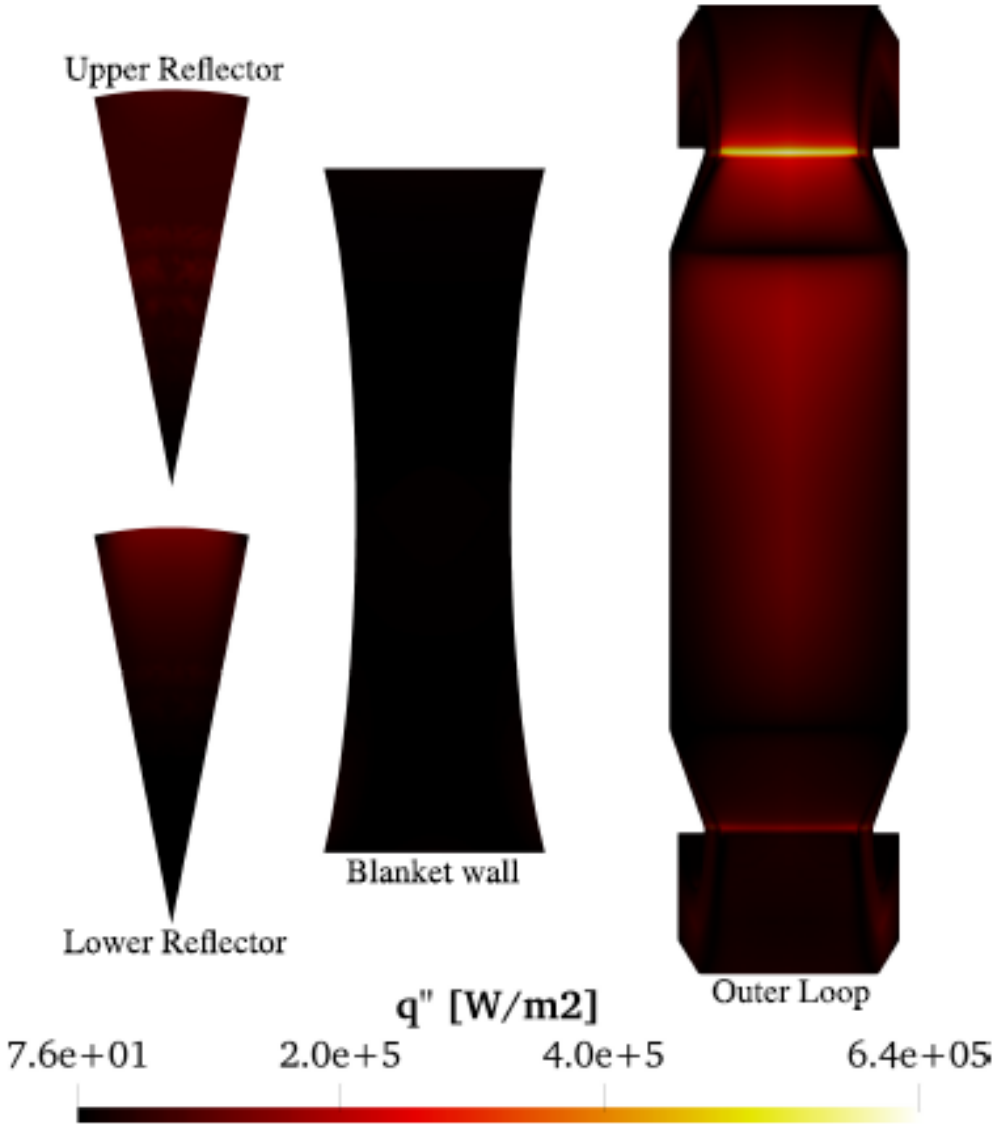


$$Q_{mix} = \sum_{i=1}^{n} (\lambda_i E_{d,i}) N_i = Q_{eff} N_{tot}$$

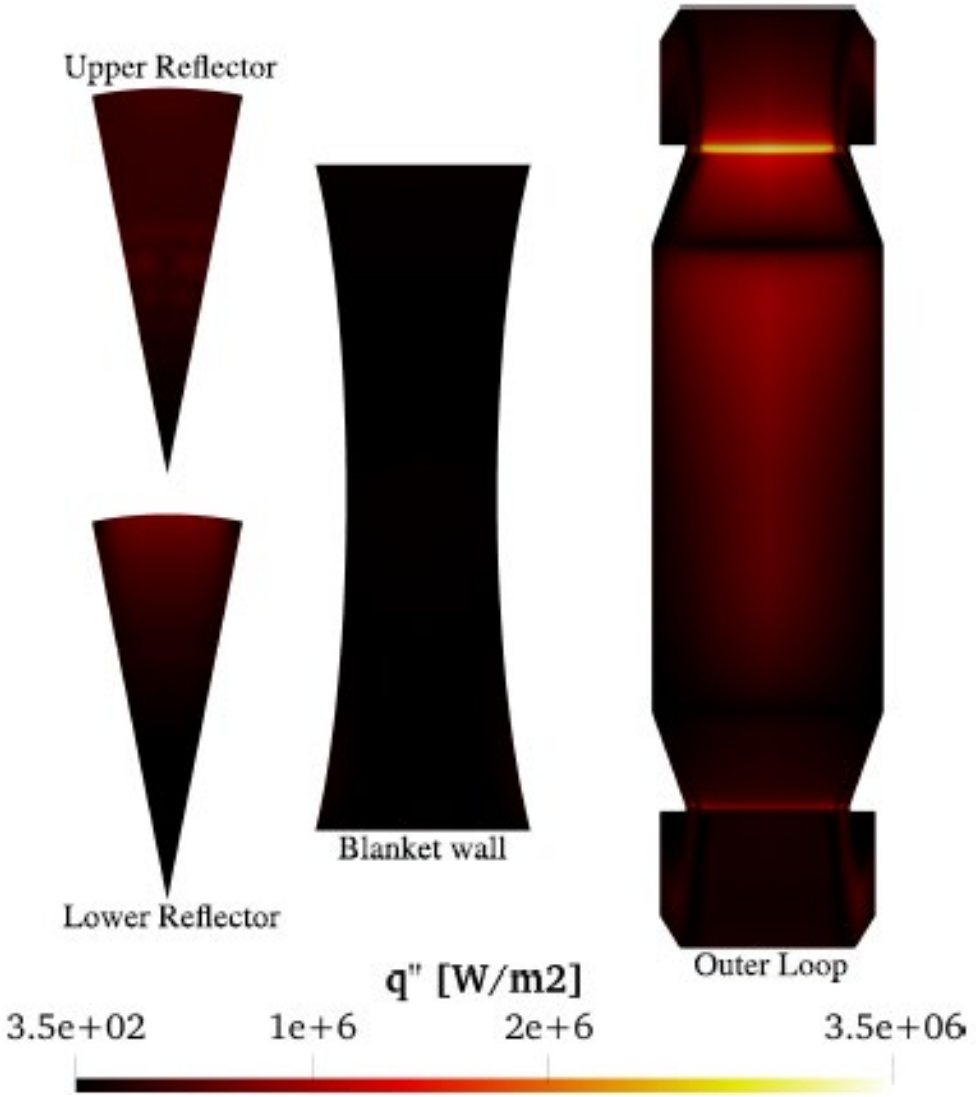


5M simulation: decay heat

5M



Metals



Conclusions

- 5M simulation: 5M concentration and deposition with clustering – both with perfect sink and deposition velocity BC
- Information on rate of deposition on the structural walls + heat decay contribution
- Steady-state approach: Deposition physics is extremely low compared to the precipitation-diffusion modelling
- Coupling with ThermoChimica can provide additional information on that since it allows to accurately reproduce the chemistry (formation and physical state of the possible species)
- But there is need to improve the database of 5M with respect to the fluoride formation species