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PSI

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Session 3-1: ESFR Core & Fuel
Coupled core T-H & neutronics simulation

ESFR-Smart Spring School - 29 -31 March, Cambridge, Zoom webinar

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Objective of the presentation

I. Importance of steady state and transient coupled simulations

II. Brief overview on interaction between neutronics and Thermal-Hydraulics (TH)

III. Selected issues of coupled modeling

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T-H & neutronics simulation: **steady state**

- **Coupling in steady state** is important from conceptual and safety perspective:
  - To assure balanced outlet fuel temperature (sodium flow orificing).
  - To identify hot spots and assess fuel performance.
  - To assure that overall reactivity introduced by increase of power or inlet sodium temperature is negative.
  - To assure sufficient shut-down reactivity margin and avoid re-criticality by cooling.
- **Cold reactor** at zero power has different reactivity than **hot reactor at zero power**.
- **Reactor at nominal power** has difference reactivity than **hot reactor at zero power**.

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T-H & neutronics simulation: **transients**

- Coupled neutronics and TH simulation should prove **acceptable behavior** of the ESFR-SMART core during **nominal and transient situation**.
- At best there should be **no chance** that transient will result in **reactivity runaway**. (Positive temperature feedbacks, like in RBMK or PHWR reactors, should be avoided)
- In transient case the tight coupling of neutronics and TH is necessary especially when both independent **reactor shut-down mechanisms fail**. *(other way the neutronics is limited to decay heat curve)*
- Should this failure by combined with, e. g., **loss-of-flow event** the resulting transient is **highly nonlinear** and requires **tight coupling of neutronics and TH**.
- Keep in mind that we speak about **double-failure**, which can be eventually acceptable for regulator because of its **low probability**.

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Interaction between Neutronics and TH

TH impacts on neutronics

Type of:

Impact

Impacted property / medium

Impact mechanism

Materials temperature

Atomic motion velocity

1. Changed microscopic cross-sections

Atomic density

2. Changed density and geometry of solids

3. Changed density of fluids

Fluids velocity

Moving of coolant atoms

Negligible impact (particle motion velocity >> fluids velocity)

Moving of fuel atoms

Drift of delayed neutron precursors (issue for MSR)

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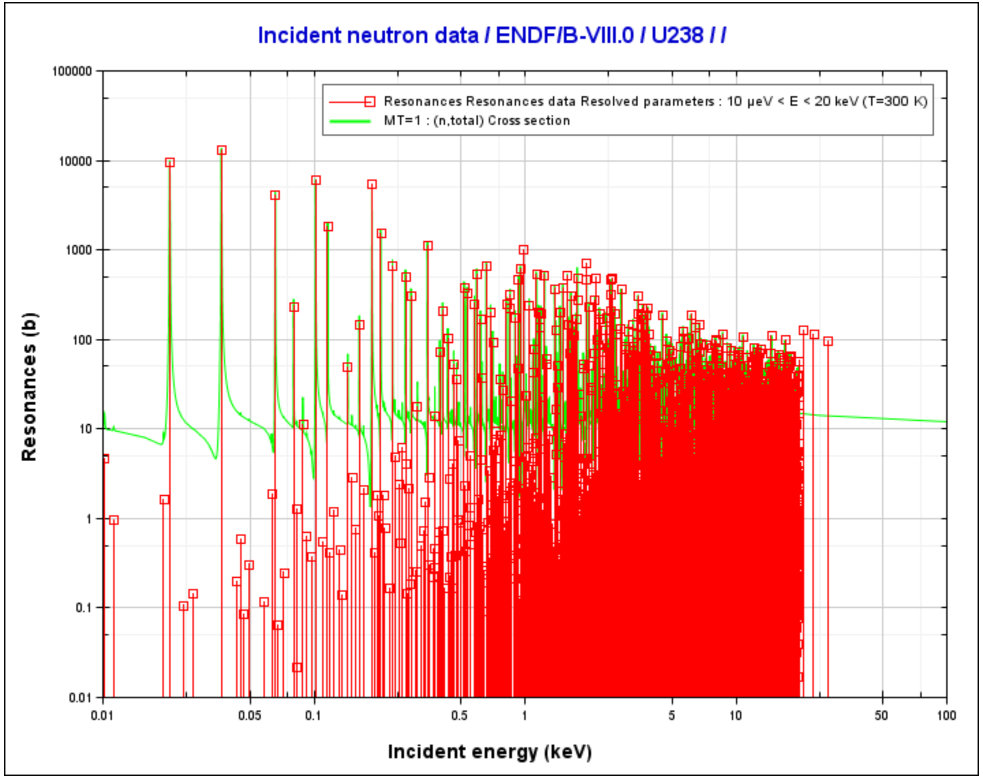
1. Changed microscopic Cross-sections (XS)

- **XS** is a measure of **probability** than neutron will interact with the atom (nucleus).
- **XS** has resonances (at certain mutual velocities the interaction probability is higher)
- **Resonances** are based on internal structure of the nucleus and more frequent for heavier elements.
- Resonances are the reason for **energetic self-shielding** and local shape of **neutron spectrum**.



https://www.oecd-nea.org/jcms/pl_39910/janis

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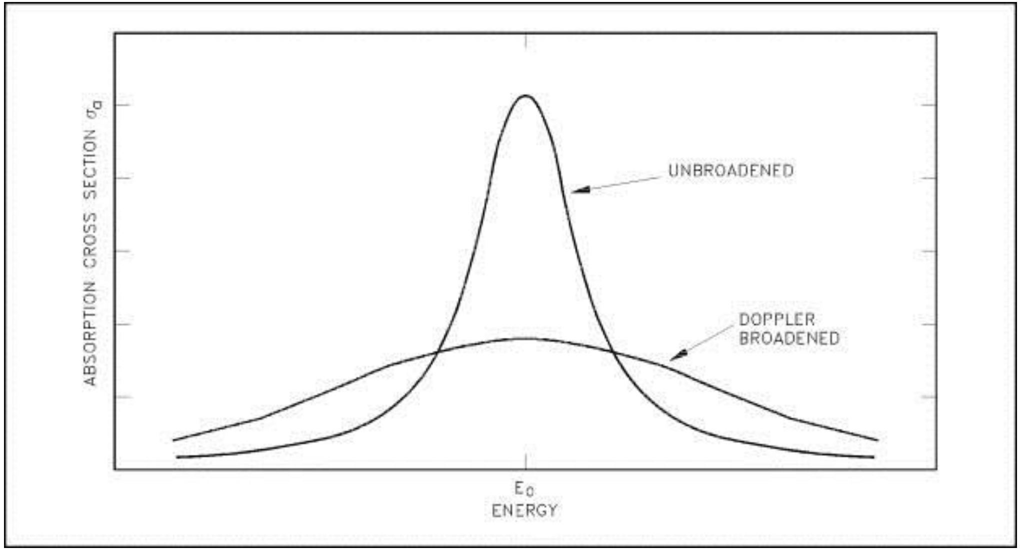
1. Changed microscopic Cross-sections (XS)

- **XS** depends on the **mutual velocity** of the nucleus and neutron.
- **Nucleus motion velocity** depends on the **material temperature**.
- Convention is so that **XS** are plotted / used as a **function of neutron velocity only**.
- The impact of **nucleus velocity** is included in the actual **XS data**. Accordingly, the nuclei thermal motion is smearing the **XS =>**
- The **Doppler-broadening** of resonances is the main cause of spectral changes and fastest mechanisms of TH impact on XS.



https://www.nuclear-power.net/glossary/doppler-broadening/

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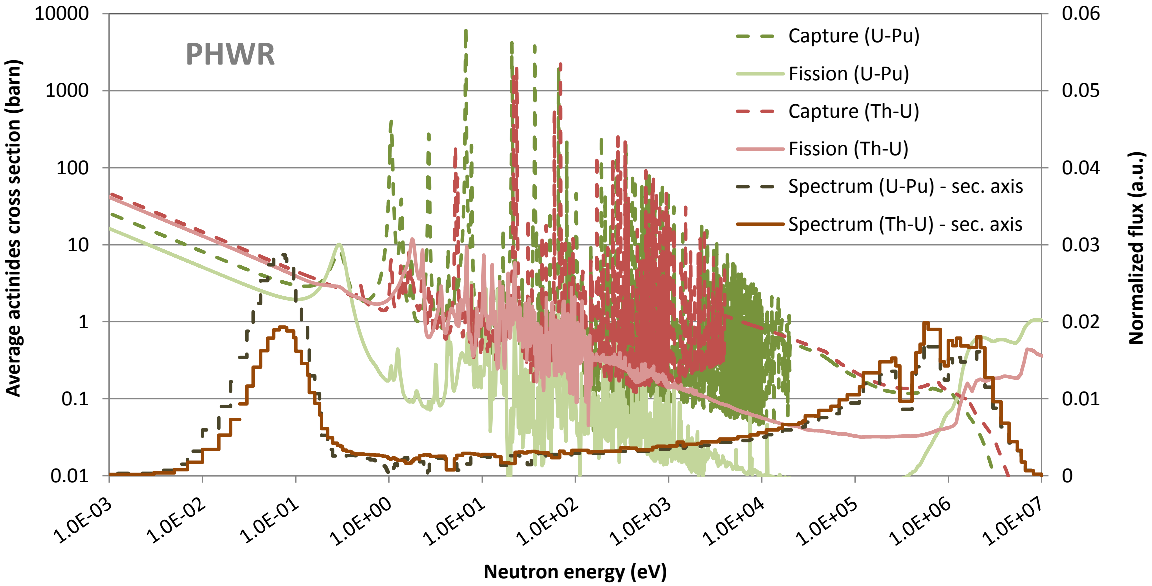
1. Changed microscopic Cross-sections (XS)

- The **impact of resonances broadening** depends on the **spectrum type**.
- In **thermal spectrum** (e.g. Pressurized Heavy Water Reactor - PHWR) it reduces the **resonance escape probability** during the neutron slowing down process.



Křepel, J., Losa, E., 2019. Closed U-Pu and Th-U cycle in sixteen selected reactors: evaluation of major equilibrium features. Ann. Nucl. Energy.

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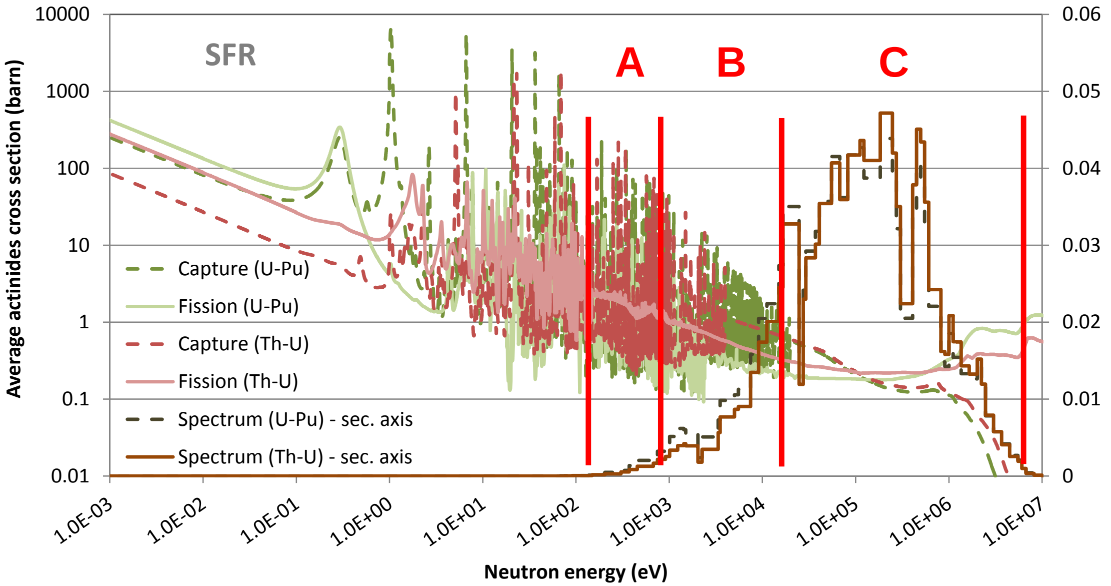
1. Changed microscopic Cross-sections (XS)

- The **impact of resonances broadening** depends on the **spectrum type**.
- In **fast spectrum** (e.g. Sodium Fast Reactor – SFR) it **increases neutron capture** in the spectrum tail and **shifts so the spectrum** towards higher energies.



Doppler broadening impact:

A Flux reduction dominates
B XS increase dominates
C Flux increase dominates

Křepel, J., et al., 2011. Comparison of safety related parameters of Generation-IV fast reactors in equilibrium closed cycle, Global 2011, Japan, Dec. 11-16,

Křepel, J., Losa, E., 2019. Closed U-Pu and Th-U cycle in sixteen selected reactors: evaluation of major equilibrium features. Ann. Nucl. Energy.

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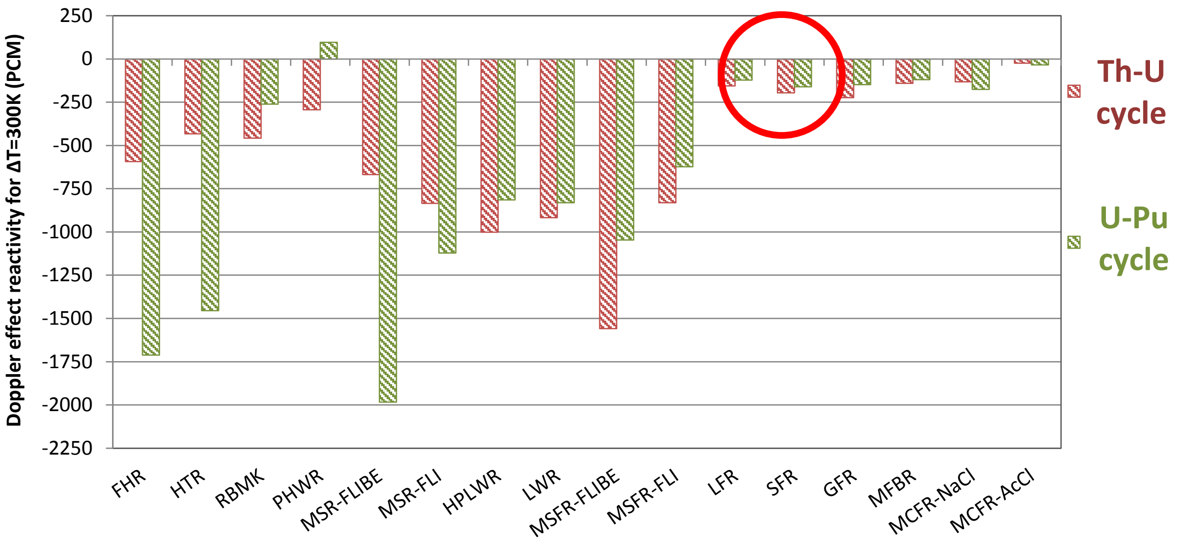
1. Changed microscopic Cross-sections (XS)

- **Doppler broadening of XS** result in **negative reactivity** practically in all reactor with substantial share of heavy nuclei with capture XS resonances (**^{238}U and ^{232}Th**).
- As an example reactivity introduced by **300K** fuel temperature increase is shown.
- *The figure shows results for **iso-breeding** fuel **composition**. It is not a value for standard fuel composition.*
- *No time to discuss PHWR. Have a look on the paper or on the fission XS resonance 2 slides above.*



Krepel, J., Losa, E., 2021, Self-sustaining breeding in advanced reactors: Characterization of selected reactors, Chapter 00123, Nuclear encyclopedia.

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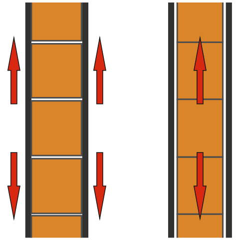
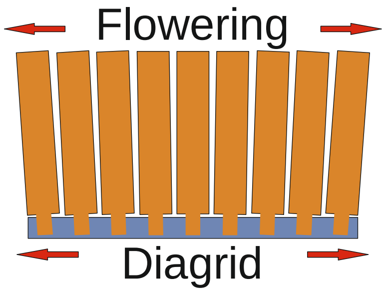
2. Changed density and geometry of solids

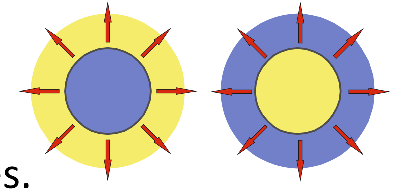
- **Temperature increase** of solid materials results in their **thermal expansion**.
- **Active core** is delimited by **fuel presence**.
- Active core **axial** expansion is driven by **fuel or cladding temperature**.
  (cladding temperature drives fuel position in case of closed gap between them)



- Active core **radial** expansion is driven by **diagrid expansion** and assemblies **flowering effect**.



- **Non-fuel** solid **materials** can expand:
  – **outwards** from the active core, e.g., **cladding** with open gap
  – **inwards** to the active core, e.g., control rods and **control rods drivers expansion**
- Expansion of **solid materials can expel fluids** from the core.
  – e. g., cladding radial expansion expels sodium from the core.
  – in rare cases it can be the opposite, e. g., fluid in expanding tubes.



Yellow: fluid, Blue: solid

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2. Changed density and geometry of solids

- **ESFR-SMART** thermal **expansion coefficients**:

1. Axial fuel expansion (inner zone).
2. Axial fuel expansion (outer zone).
   (increased cladding and sodium mass)
3. Axial cladding expansion (inner z.).
4. Axial cladding expansion (outer z.).
   (decreased cladding mass)
5. Radial cladding expansion inner z.).
6. Radial cladding expansion (outer z.).
   (decreased sodium mass)
7. Diagrid expansion
   (increased sodium mass)

8. Control rods drivers expansion (not shown) introduces negative reactivity.

ESFR-SMART, Deliverable D1.2.2, Analysis of safety and performance parameters of the ESFR-SMART core at end of cycle.

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3. Changed density of fluids

- Fluids can have 3 functions in the active core:
  1. **Coolant**
  2. **Moderator**
  3. **Fuel** (in MSR case)
- **Fluid temperature** increase does **not** change the core **geometry,**
- **but it reduces** density and so **scattering and capture XS** of the fluid.
  (and fission XS in case of fluid fuel MSR)
- Reduced capture XS = always positive reactivity
  Reduced scattering XS = spectrum hardening (different reactivity in different spectra)

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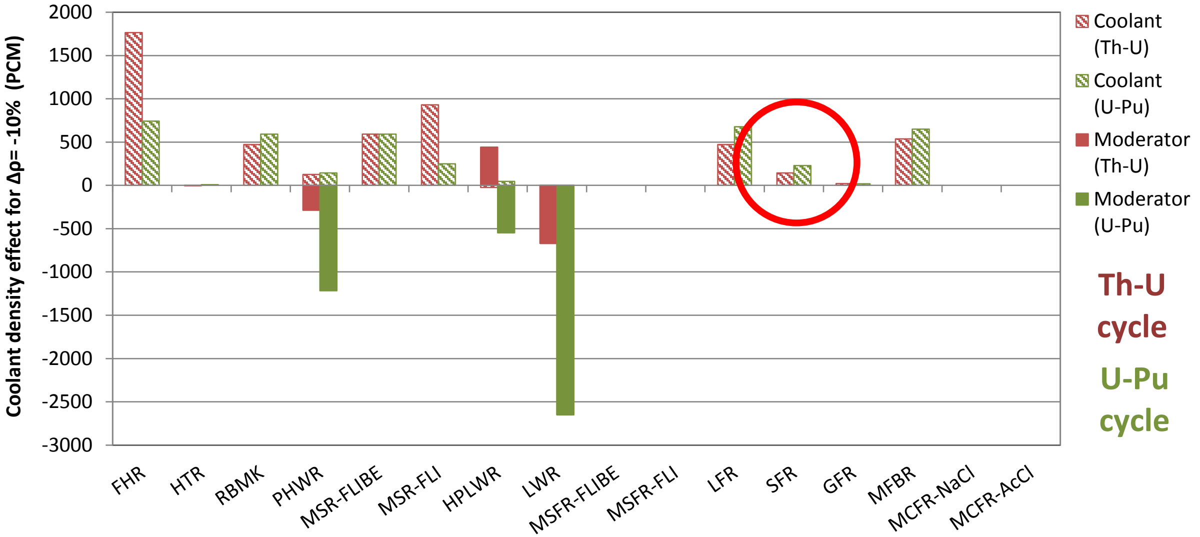
3. Changed density of fluids

- **Decreased density** result typically in **positive reactivity.**
  Only for moderating fluid it is negative (reduced scattering XS dominate).

- As an example **10% density reduction** is shown. *(infinite lattice simulation = 0 for hom. reactors)*

- *The figure shows results for **iso-breeding** fuel **composition**. It is not a value for standard fuel composition.*



- *In MSR-FLI and MSR-FLIBE two effects take a part: reduced salt capture and changed fuel-to-moderator ratio, Doppler effect is not included.*

Krepel, J., Losa, E., 2021, Self-sustaining breeding in advanced reactors: Characterization of selected reactors, Chapter 00123, Nuclear encyclopedia.

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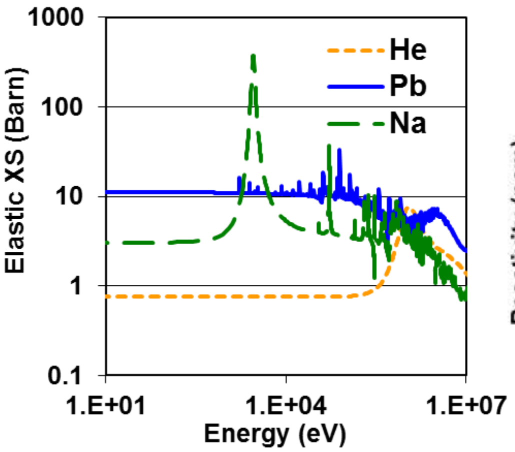
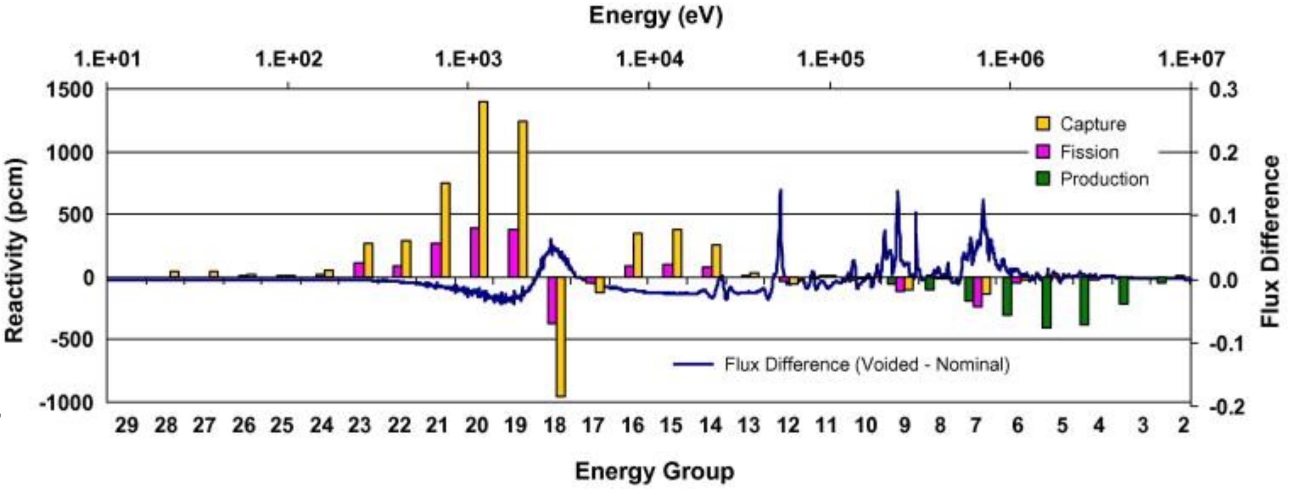
3. Sodium density reduction

- Sodium has few resonances, biggest at 3KeV. Other way its scattering XS is quite low. *(It is comparable to deuterium. Sodium is not a moderator because its mass and capture prob. is higher.)*
- Sodium density reduction (voiding) locally change the spectrum and results in decrease of fission and capture rate and increased neutron leakage:

CP ESFR *(working horse core)*	$\Delta\rho$		$\Delta\rho_L$		$\Delta\rho_C$		$\Delta\rho_F$	$\Delta\rho_P$
	2071.0	=	-620.3	+	3788.3	+	666.5	-1763.5





Sun K., et al., 2011, Void reactivity decomposition for the Sodium-cooled Fast Reactor in equilibrium fuel cycle, ANE, vol. 38, pp. 1645-1657.

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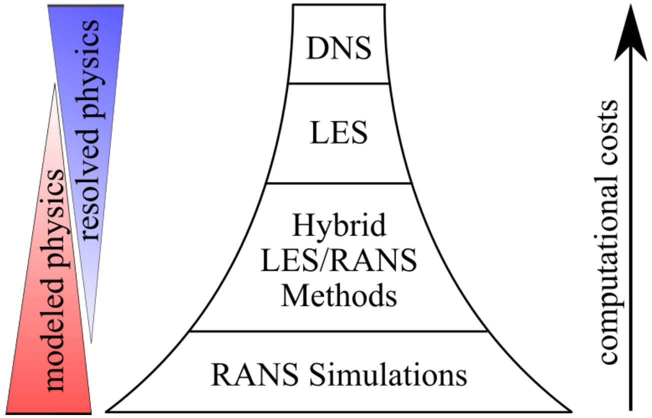
Neutronics X TH solvers

- **Deterministic approach:**
  1. **Multi-group XS** are generated by a **cell / lattice code** for given temperatures and compositions. Alternatively, a multi-group XS database is prepared for many temperatures and compositions.
  2. XS are applied in **nodal solver** based, e.g., on diffusion or simplified transport and regular square or Hex-Z nodes.
  3. XS are applied in solvers based on Method of characteristic (**MOC**), Finite element method (**FEM**), Finite volume method (**FVM**), Finite difference method (**FDM**).
- **Stochastic approach:**
  1. Monte-Carlo method for neutron transport direct solution using point-wise XS.

- **CFD approach:**



Xiao H., 2018, Quantification of Model Uncertainty in RANS Simulations: A Review

- **System code with 1D channel-wise resolution:**
  (TRACE, RELAP, etc.)

- **Core only 1D channel-wise resolution**

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Coupling of Neutronics & TH solvers

1. **Ultimate solution:** **CFD** solver can be tightly coupled with **Monte Carlo** solver.
   In this most exact but also most demanding case point-wise XS are used.
2. **Challenging solution:** **CFD** solver can be tightly coupled with deterministic **MOC, FEM, FVM, or FDM** solver.
3. **Standard solution:** **1D channel-wise system code** can be coupled with deterministic **nodal solver** (core represented by rigid nodal 3D geometry).
4. **Simplified solution:** **1D channel-wise system code** can be coupled with point kinetics model (neutronics represented only by integral properties).

Coupling interface: 1) none* – direct use of temperature field and atomic concentrations
2&3) temperature dependent local **multi-group XS** or temperature and atomic concentration dependent **multi-group XS** library.
4) temperature dependent **distributed coefficients** or just **integral coefficients**.

** Actually, even the XS for Monte Carlo code needs to be "prepared" for different temperatures.*

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Didn’t we missed something?

1. Modeling of **thermal expansions** is necessary to couple neutronics & TH.
2. The **Thermal-Mechanics model** also has several possible level of accuracy.
3. Usually the **Multi-group XS** (as well as the point-kinetics coefficients) are generated by a cell / lattice code (or full core code) using “manually” **expanded geometry**.
4. **Thermal-Mechanics model** is often the one **mostly restricted** by the selected simulation approach and geometry. *(e.g, nodal solvers cannot model flowering)*
5. However, the two major players: **Doppler effect and Sodium density effect do not change** the geometry.

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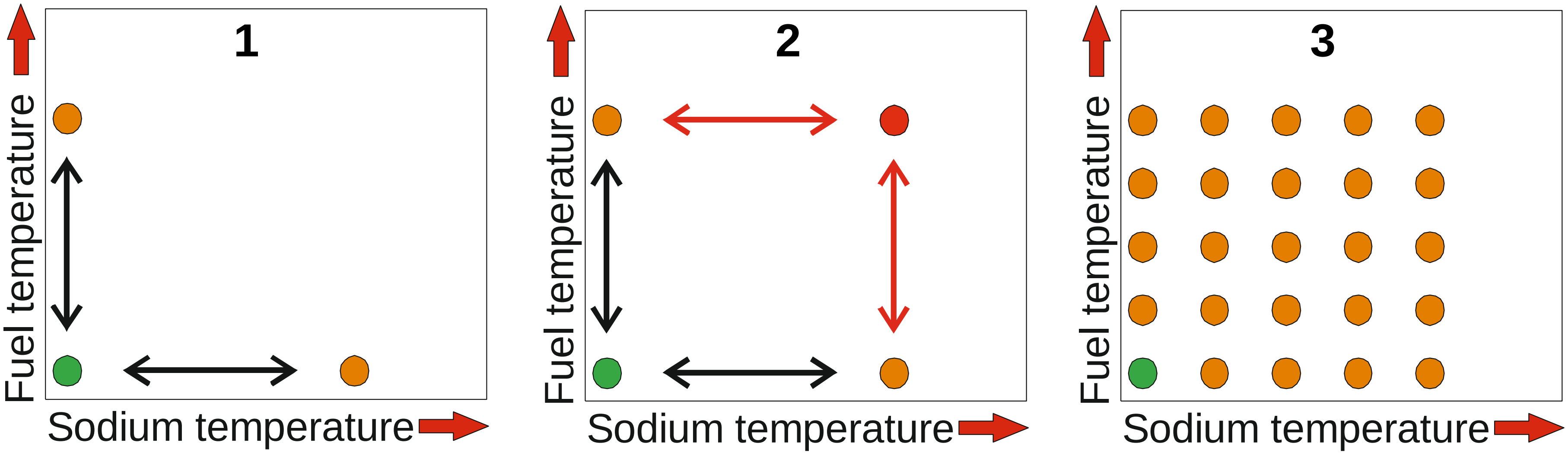
Coupling through: Multi-group XS or coefficients

The major players: Doppler effect and Sodium density effect are **fairly independent**.

1. Accordingly, **multi-group XS** or coefficient are often based on **nominal value** and **derivatives**. Actual XS value is obtained by linear and logarithmic interpolations.
2. More precise would be **bi-interpolation** based on four values (needs 1 more point).
3. Often also tabulated multi-group XS and interpolation are used.



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Issue with reactivity coefficients

- **Multi-group XS** are not perfect, but capture well the **local conditions**.
- Coupling through Multi-group XS **addresses** possible **changes in flux shape and spectrum**.
- **Point kinetics** assumes that
  1) flux can be separated into amplitude and shape function
  2) and the **shape function is constant during transient**.

– To illustrate that let us use one group neutron flux:

$$\Phi\left(\vec{r},t\right)=vn\left(t\right)\Psi\left(\vec{r}\right)$$

where v is the neutron velocity, $n\left(t\right)$ neutron density, $\Psi\left(\vec{r}\right)$ the flux shape function.

– During the **unprotected loss of flow** sodium boiling can occur.

– **Shape function can change** and application of point kinetics is thus questionable.

– To address it, the **additivity and correlation** of partial effect should be checked.

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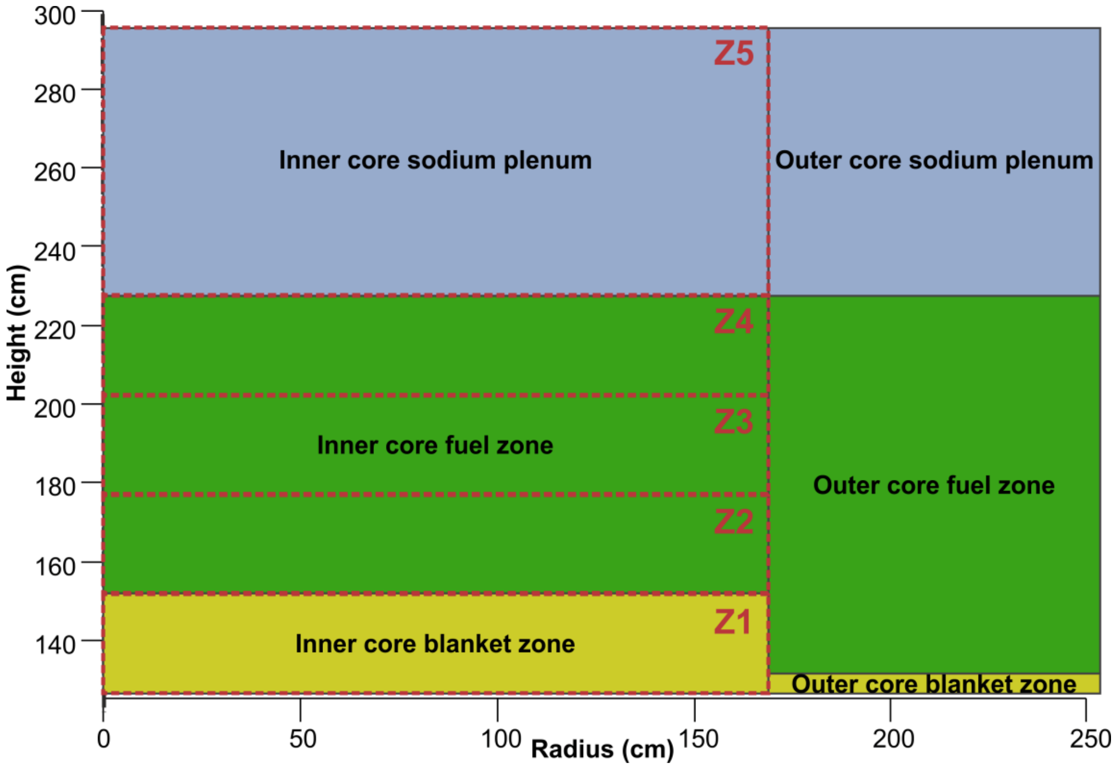
ESFR-SMART core division into zones

- Mutual inter dependence and additivity was checked using 5 axial zones in the internal fuel zone of ESFR-SMART core.



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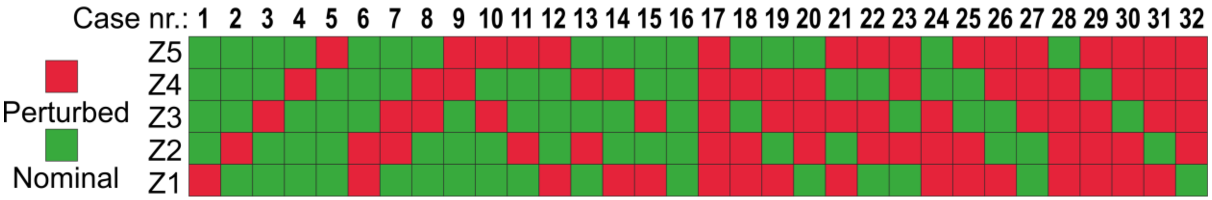
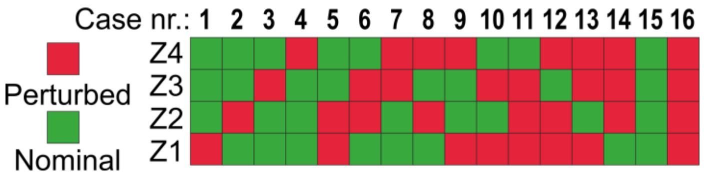
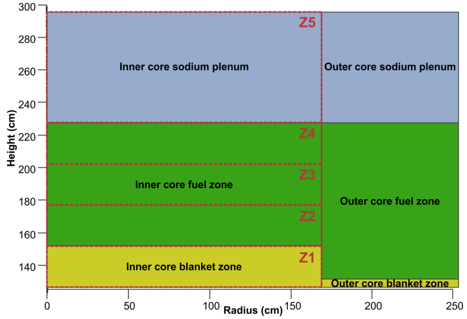
Perturbation of the zones

- For sodium void effect all 5 zones were used.
- There are 32 possible voiding option.



- For other effect: **Fuel temperature, Fuel density, and Cladding density** only the 4 core zones have been used, resulting in 16 combinations.





Krepel, J., et al., 2021, SPATIAL INTERDEPENDENCE OF SAFETY RELATED EFFECTS IN ESFR-SMART CORE, FR21 (FR22) proceedings.

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Void mutual inter dependence

- The void effect is positive in the core and negative in the sodium plenum.
- **strongest** mutual inter **dependence** was identified for **upper core part Z4 and plenum Z5**.

Void effect	**Impact of other zones on the main zone effect in %**														
Main Zone	**2 zones** (e.g. Z1+Z2)				**3 zones** (e.g. Z1+Z2+Z3)						**4 zones**				**5 zones**
Z1	Z2	Z3	Z4	Z5	Z2,Z3	Z2,Z4	Z2,Z5	Z3,Z4	Z3,Z5	Z4,Z5	Z2,Z3,Z4	Z2,Z3,Z5	Z2,Z4,Z5	Z3,Z4,Z5	Z2,Z3,Z4,Z5
7.4 (PCM)	-2	-24	-13	6	4	-5	22	-29	4	5	-19	15	21	3	14
Z2	Z1	Z3	Z4	Z5	Z1,Z3	Z1,Z4	Z1,Z5	Z3,Z4	Z3,Z5	Z4,Z5	Z1,Z3,Z4	Z1,Z3,Z5	Z1,Z4,Z5	Z3,Z4,Z5	Z1,Z3,Z4,Z5
266.0 (PCM)	0	9	1	5	9	1	6	10	-1	7	10	-1	8	-1	-1
Z3	Z1	Z2	Z4	Z5	Z1,Z2	Z1,Z4	Z1,Z5	Z2,Z4	Z2,Z5	Z4,Z5	Z1,Z2,Z4	Z1,Z2,Z5	Z1,Z4,Z5	Z2,Z4,Z5	Z1,Z2,Z4,Z5
470.6 (PCM)	0	5	3	-9	5	3	-9	8	-13	-8	8	-13	-8	-12	-12
Z4	Z1	Z2	Z3	Z5	Z1,Z2	Z1,Z3	Z1,Z5	Z2,Z3	Z2,Z5	Z3,Z5	Z1,Z2,Z3	Z1,Z2,Z5	Z1,Z3,Z5	Z2,Z3,Z5	Z1 Z2,Z3,Z5
137.9 (PCM)	-1	2	12	-68	2	11	-68	14	-65	-62	13	-65	-62	-62	-62
Z5	Z1	Z2	Z3	Z4	Z1,Z2	Z1,Z3	Z1,Z4	Z2,Z3	Z2,Z4	Z3,Z4	Z1,Z2,Z3	Z1,Z2,Z4	Z1,Z3,Z4	Z2,Z3,Z4	Z1 Z2,Z3,Z4
-669.4 (PCM)	0	-2	7	14	-2	6	14	10	12	22	10	11	21	26	26

Krepel, J., et al., 2021, SPATIAL INTERDEPENDENCE OF SAFETY RELATED EFFECTS IN ESFR-SMART CORE, FR21 (FR22) proceedings.

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Doppler effect mutual inter dependence

- The Doppler effect (+1000K) is generally negative.
- Mutual inter dependence is much weaker (smaller flux shape changes).

Doppler effect	Impact of other zones on the main zone effect in %						
Main Zone	**2 zones** (e.g. Z1+Z2)			**3 zones**			**4 zones**
Z1	Z2	Z3	Z4	Z2,Z3	Z2,Z4	Z3,Z4	Z2,Z3,Z4
-55.3 (PCM)	-16	4	10	0	1	3	0
Z2	Z1	Z3	Z4	Z1,Z3	Z1,Z4	Z3,Z4	Z1,Z3,Z4
-75.9 (PCM)	-12	-7	-1	-10	-8	-8	-10
Z3	Z1	Z2	Z4	Z1,Z2	Z1,Z4	Z2,Z4	Z1,Z2,Z4
-91.7 (PCM)	2	-6	2	4	-2	-4	-4
Z4	Z1	Z2	Z3	Z1,Z2	Z1,Z3	Z2,Z3	Z1,Z2,Z3
-57.3 (PCM)	10	-2	3	14	3	1	2

Krepel, J., et al., 2021, SPATIAL INTERDEPENDENCE OF SAFETY RELATED EFFECTS IN ESFR-SMART CORE, FR21 (FR22) proceedings.

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Fuel density effect mutual inter dependence

- Fuel density effect (10% density reduction) is generally negative in fissile zone.
- Fuel density effect has medium mutual inter dependence, which is driven by flux shape.

Fuel density effect	Impact of other zones on the main zone effect in %						
Main Zone	2 zones (e.g. Z1+Z2)			3 zones			4 zones
Z1 6.9 (PCM)	Z2	Z3	Z4	Z2,Z3	Z2,Z4	Z3,Z4	Z2,Z3,Z4
	-3	5	6	2	0	5	5
Z2 -418.2 (PCM)	Z1	Z3	Z4	Z1,Z3	Z1,Z4	Z3,Z4	Z1,Z3,Z4
	0	-9	-4	-9	-4	-17	-17
Z3 -509.0 (PCM)	Z1	Z2	Z4	Z1,Z2	Z1,Z4	Z2,Z4	Z1,Z2,Z4
	0	-8	-7	-8	-7	-18	-18
Z4 -354.8 (PCM)	Z1	Z2	Z3	Z1,Z2	Z1,Z3	Z2,Z3	Z1,Z2,Z3
	0	-5	-10	-5	-10	-20	-20

Krepel, J., et al., 2021, SPATIAL INTERDEPENDENCE OF SAFETY RELATED EFFECTS IN ESFR-SMART CORE, FR21 (FR22) proceedings.

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Cladding density effect mutual inter dependence

- Cladding density effect (10% density reduction) is generally positive.
- It has mild mutual inter dependence, which is driven by flux shape.

Cladding density effect	Impact of other zones on the main zone effect in %						
Main Zone	2 zones (e.g. Z1+Z2)			3 zones			4 zones
Z1 11.2 (PCM)	Z2	Z3	Z4	Z2,Z3	Z2,Z4	Z3,Z4	Z2,Z3,Z4
	6	8	4	12	7	1	8
Z2 107.5 (PCM)	Z1	Z3	Z4	Z1,Z3	Z1,Z4	Z3,Z4	Z1,Z3,Z4
	1	2	0	3	1	3	4
Z3 176.8 (PCM)	Z1	Z2	Z4	Z1,Z2	Z1,Z4	Z2,Z4	Z1,Z2,Z4
	0	1	1	2	1	3	3
Z4 63.9 (PCM)	Z1	Z2	Z3	Z1,Z2	Z1,Z3	Z2,Z3	Z1,Z2,Z3
	1	1	4	1	3	5	5

Krepel, J., et al., 2021, SPATIAL INTERDEPENDENCE OF SAFETY RELATED EFFECTS IN ESFR-SMART CORE, FR21 (FR22) proceedings.

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Additivity of the effect in active core

- Sodium void effect, Fuel temperature, Fuel density, and Cladding density are **all reasonable additive in the active core**

Additivity in the core	Z1234	Z1+Z234	Z2+Z134	Z3+Z124	Z4+Z123	Z12+Z34	Z13+Z24	Z14+Z23	Z1+2+3+4
Sodium void effect	**923.2**	924.6	895.9	884.7	904.7	898.0	883.2	904.5	881.9
Difference in %	**reference**	0.2	-3.0	-4.2	-2.0	-2.7	-4.3	-2.0	-4.5
Fuel temperature effect	**-275.9**	-275.7	-283.7	-279.6	-274.9	-273.4	-281.1	-280.4	-280.3
Difference in %	**reference**	-0.1	2.9	1.3	-0.3	-0.9	1.9	1.7	1.6
Fuel density effect	**-1166.0**	-1166.4	-1237.6	-1256.6	-1236.7	-1238.1	-1256.3	-1236.4	-1275.1
Difference in %	**reference**	0.0	6.1	7.8	6.1	6.2	7.7	6.0	9.4
Cladding density effect	**366.1**	365.1	362.0	360.5	363.2	362.5	360.6	362.2	359.3
Difference in %	**reference**	-0.3	-1.1	-1.5	-0.8	-1.0	-1.5	-1.1	-1.9

Krepel, J., et al., 2021, SPATIAL INTERDEPENDENCE OF SAFETY RELATED EFFECTS IN ESFR-SMART CORE, FR21 (FR22) proceedings.

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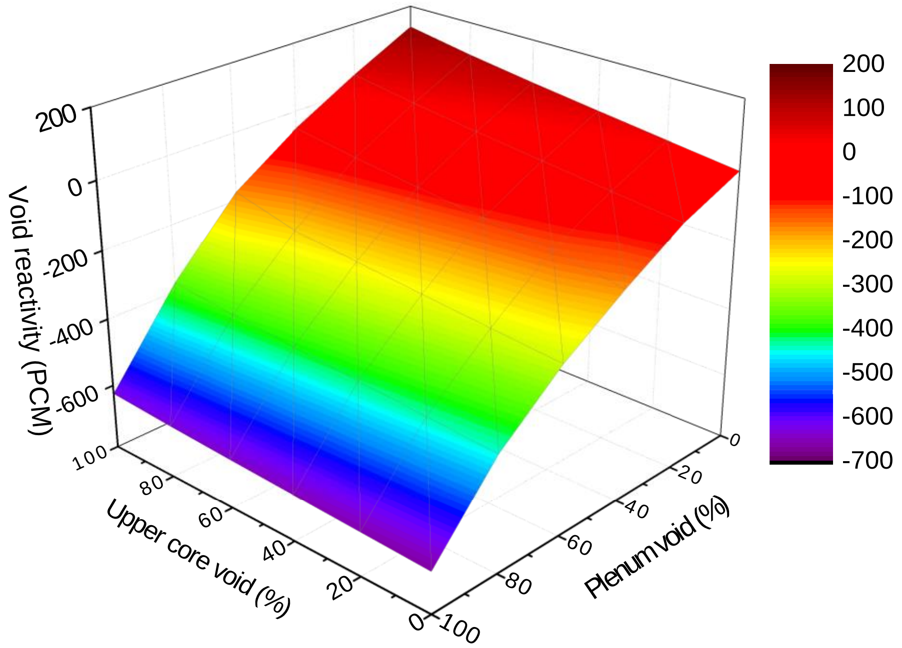
Void in upper part

- Sodium void effect is **not really additive for upper fuel Z4 and sodium plenum Z5 zones.**
- Sodium plenum void increases neutron leakage and is not linear =>
- However summation of two effects in Z4 and Z5 is more conservative than bi-linear interpolation between 4 points. *(only because of compensating effects)*



Additivity with plenum	Z2345	Z2+Z345	Z3+Z245	Z4+Z235	Z5+Z234	Z23+Z45	Z24+Z35	Z25+Z34	Z2+3+4+5
Sodium void effect	73.5	76.1	130.5	159.3	247.8	135.1	164.6	235.8	205.123
Difference in %	reference	3.5	77.5	116.7	237.1	83.8	123.9	220.7	179.0

Krepel, J., et al., 2021, SPATIAL INTERDEPENDENCE OF SAFETY RELATED EFFECTS IN ESFR-SMART CORE, FR21 (FR22) proceedings.

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Summary

- Coupled neutronics & TH simulation are important for conceptual studies as well as for safety assessment.
- Accuracy of the simulation tool should be selected according to the importance of the results.
- Standard solution uses multi-group XS as the coupling between TH & neutronics solver. *(the solver uses prepared XS to calculate flux shape)*
- Transients without sodium boiling, can be well addressed by TH & point kinetics.
- In transients with sodium boiling, which are CPU demanding from TH perspective, point kinetics is less precise and the related CPU savings are less important.

Thank you for your attention.