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SIMULATIONS OF SOME STRUCTURAL MATERIALS BEHAVIOUR UNDER NEUTRON IRRADIATION

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- Material performance under neutron irradiation - one of the most important factors in assessing the candidate materials for new reactor concepts;
- Large number of studies have been reported regarding their behavior under different neutron spectra and irradiation temperatures.

- **Molybdenum alloys** - investigated extensively being considered as promising materials able to withstand a harsh environment due to their characteristics:
  - *high strength and melting point,*
  - *high thermal conductivity,*
  - *good corrosion resistance against liquid metals;*

- **Vanadium alloys** are recognized as attractive structural materials for fusion systems due to:
  - *mechanical tolerance to neutron damage,*
  - *high temperature strength, low long-term activation*
  - *low decay heat.*

- *preliminary analysis of their behavior under neutron irradiation in a Lead-cooled Fast Reactor (the ALFRED Demonstrator) have been performed.*

- The purpose of the present work is to investigate the impact of these alloys if used as material for fuel claddings on the reactor reactivity as well as to obtain information about the changes in their isotopic composition with irradiation.

- **The reference active core configuration of ALFRED Demonstrator was developed in the Seventh Framework Programme (FP7) LEADER project.**

Reactor Configuration and Computational Tools

- ALFRED is a critical reactor (300 MWth) for the demonstration of Lead-cooled Fast Reactor Technology;
- the reference core is MOX fuelled (hexagonal lattice) with two enrichments zones and it is provided with a control system (12 rods) used for both normal control of the reactor and for SCRAM in case of emergency and a safety system (4 rods) used only for SCRAM. A schematic view of the active core is presented in Fig. 1.

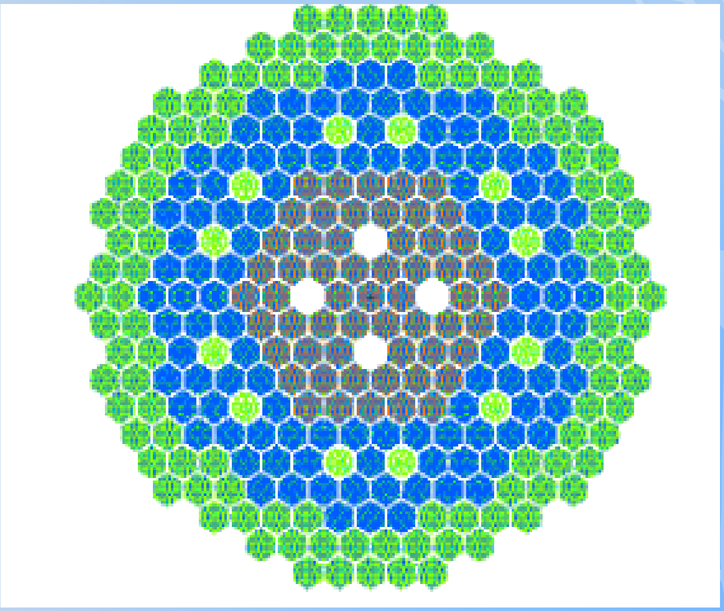

Fig. 1. *Reference core configuration*

Computational tools:

1) MCNPX – used for criticality simulations and evaluation of the neutron flux in the fuel claddings using JEFF 3.1 neutron cross-section library. The actual, detailed geometry of the whole reactor system has been modelled using MCNPX capabilities (Fig.2).

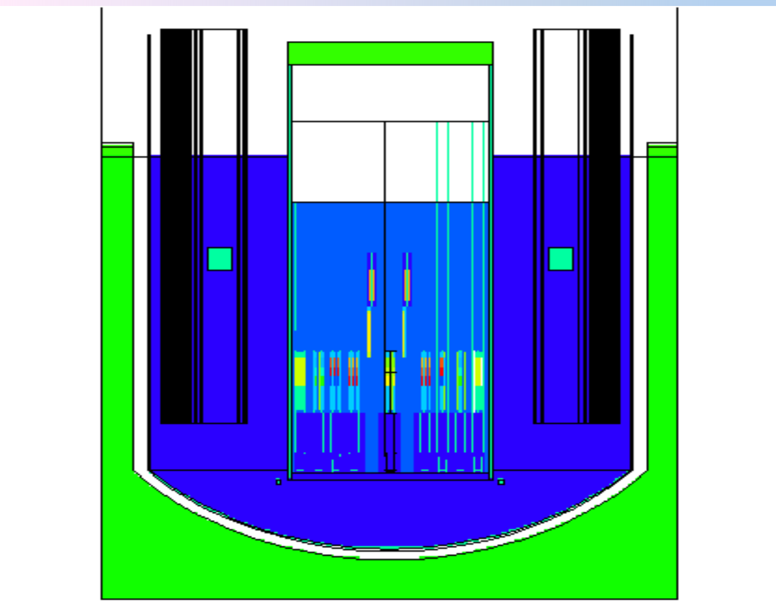

Fig.2. *MCNPX model of the reactor*

2) FISPACT code - used to evaluate the activity, the isotopic inventory and the hazard factors for each alloy used as fuel cladding based on the flux-spectrum computed by MCNPX in the respective material.

Molybdenum Alloys

- Mo-TZM (containing 0.55% Ti, 0.12% Zr and 0.04% C (wt %)),
- Mo-Re 5%
- Mo-Re 47.2%.

a) Criticality computations

(evaluation of the effect of using these alloys as fuel cladding materials on the neutron economy of the reactor)

Table 1 shows the k_{eff} values for each case along with the k_{eff} obtained for the reference ALFRED core configuration where the fuel cladding material is 15-15 Ti stainless steel.

Tab. 1. *k-effective values for molybdenum alloys*

Cladding	TZM	Mo-Re 5%	Mo-Re 47%	15-15 Ti
k_{eff}	0.9953	0.9823	0.8750	1.0805

- the reactor *could become strongly sub-critical when using Mo-Re alloys having a high concentration of Re.*

- **This behaviour is mainly due to the large neutron absorption cross-sections of both Mo and Mo-Re47% in the energy range 1eV – 1keV as can be observed in Fig. 3.**

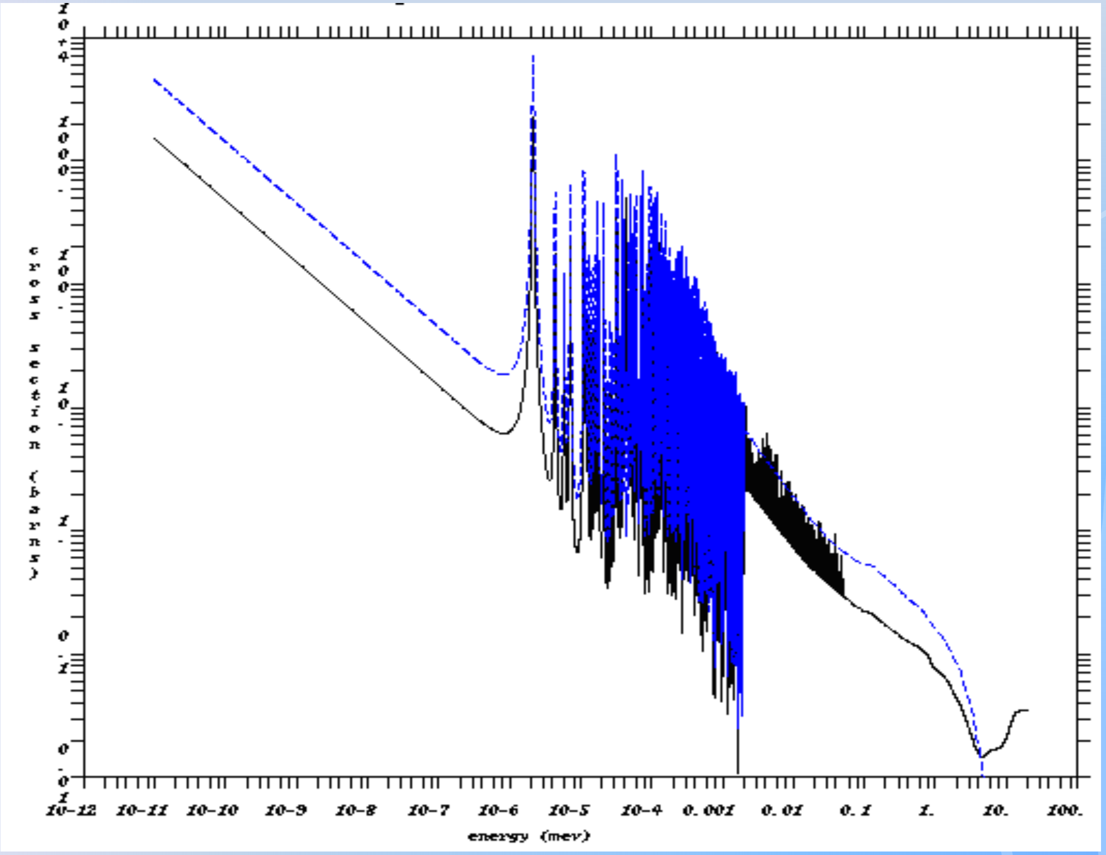

Fig. 3. *Neutron absorption cross-sections for Mo and Mo-Re47%.*

- **Their impact is also reflected in the average neutron flux-spectra evaluated in the fuel claddings for each Mo alloy, Fig. 4.**

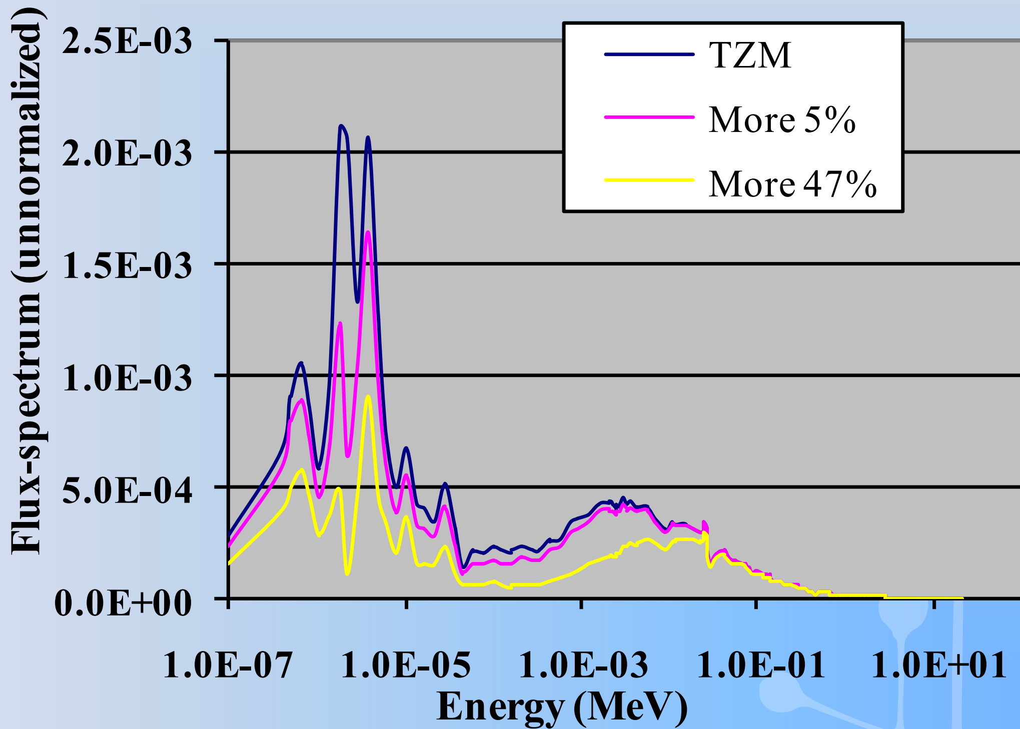

Fig. 4. *Neutron flux-spectra.*

- It should be also noticed that the high level of neutron absorption affects the evaluation of the damage produced by neutrons (DPA) in these alloys;
- Moreover, the transmutation processes affect the DPA computed values because of the alloy composition changes with irradiation;
- the MCNPX evaluation of the damage cross sections are based on the contributions (by weight) of the individual isotopes;.

The polyatomic DPA model results can be significantly different than the sum of monoatomic displacement terms;

- *if these alloys are intended to be used in the active core of a nuclear reactor* ***provisions should be taken with regards to the control rod system reactivity or the fuel enrichments during the design stage of the reactor;***
- It seems that from neutronic point of view, *the use of Mo alloys with a high concentration of Re inside the active core should be treated with caution and more detailed analyses have to be performed.*

(b) **Energy deposition in the claddings** - higher Re concentration leads to an increase of the neutron and gamma heating as presented in Table 2. The values have been obtained in the central fuel assembly using MCNPX code.

Tab. 2. *Energy deposition for molybdenum alloys*

Heating (MeV/g/ n-source)	TZM	Mo- Re5%	Mo-Re47%	15-15 Ti
	1.16E-07	1.54E-07	3.65E-07	1.47E-07

The results show that **the heating value in case of *MO-Re47%* alloy is almost *2.5 times higher than for reference Ti 15-15 steel*** which means that the lead coolant should remove the supplementary heat and additional thermal-hydraulics studies should be performed.

(c) Estimations of *the activation and isotope inventories of the fuel claddings*

(needed as input for further analyses regarding the radioprotection and waste characterization and disposal).

The computational steps consisted in:

- computation of the average neutron flux *using MCNPX* in the fuel claddings - neutron flux used *in the FISPACT* code in order to evaluate the activation and the isotopic compositions of the Mo alloys after 5 years (the maximum residence time of the fuel in the core).

- The total activities (Bq/kg) obtained for Mo-TZM, Mo-Re5% and

Mo-Re47% are of 2.92E+14, 4.20E+14 and 1.24E+15 respectively and they show an increase with Re concentration.

- The beta decay is the main contributor and, together with the alpha decay should be taken into consideration (from personnel radioprotection point of view) during handling and transportation.
- Even after 100 cooling years, the total activities are still high (order of 10^{10} Bq/kg) and the clearance index remains also enough high due to long-lived isotopes as

$$^{93}Mo \quad ^{93m}Nb \quad ^{99}Tc \quad ^{91}Nb$$

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- *The changes of Mo alloys isotopic composition* with irradiation have been extensively studied with respect to their impact on the crystallographic structure and subsequently on the mechanical, thermal, etc. properties;

- In the case of Mo-Re alloys, besides the changes in the Mo concentration and the formation of some elements as Zr, Nb or Tc through various reaction channels, one could observe a *significant decrease of rhenium mass, an increase of tungsten* concentration as well as the formation and the increase of osmium mass with irradiation.

- Also, the transmutation process makes more difficult the accurate evaluation of the neutron irradiation damage which value is one of the main constraints during the design stage of the reactor.

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Vanadium Alloys

- scientist's efforts are focused on the improvement of the vanadium alloys microstructure either starting from the reference V -4Cr -4Ti alloy or by considering new alternative compositions or fabrication routes.
- One alternative envisaged for better performances versus high temperatures and for irradiation damage reduction was *yttrium alloying*.
- three vanadium alloys (V-4Cr-4Ti, V-4Cr-4Ti-0.15Y and V-4Cr-4Ti-0.5Y) have been considered as fuel claddings material for ALFRED reactor.
- The same computational steps as for molybdenum alloys have been performed.

(a) Table 3 - *the multiplication factors* MCNPX code for each case.

Tab. 3. *k-effective values for vanadium alloys.*

	V-4Cr-4Ti	V-4Cr-4Ti-0.15Y	V-4Cr-4Ti-0. 5Y	15-15 Ti
k_{eff}	1.08751	1.08754	1.08711	1.08050

- The use of vanadium alloys as cladding material leads to an increase of the reactivity (~ 700 pcm) which can be controlled/compensated either by the control rods system or by acting on the fuel enrichment values.

(b) The values of the energy deposition in the fuel claddings of the central fuel assembly (Table 4) do not show significant differences among the vanadium alloys investigated; a slight increase which could be due to a higher concentration of yttrium is observed.

Heating (MeV/g/ n-source)	V-4Cr-4Ti	V-4Cr-4Ti-.15Y	V-4Cr-4Ti-.5Y	15-15 Ti
	1.151E-07	1.152E-07	1.155E-07	1.473E-07

- The heating values of vanadium alloys are lower than the value obtained for the reference Ti 15-15 steel used in the design of ALFRED reactor.

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(c) The changes in the elemental composition of the vanadium alloys at various irradiation time steps (1 year, 3 years and 5 years) have been computed using the same methodology as for molybdenum alloys;

- a significant increase of chromium concentration after 5 years irradiation.
- *the burnup of vanadium with irradiation time should be also noted.*
- The total activity after 5 years irradiation lies between 2.91 – 2.97E+14 Bq/kg for the vanadium alloys and has as main contributor the beta decay.
- *The alloys containing yttrium shows higher values for the ingestion and inhalation hazard factors mainly due to the yttrium and strontium long-lived isotopes which are among the main dominants even after 100 years of cooling.*
- Even so, vanadium alloys presents a low long-term activation their total activities after 100 years cooling being much lower (almost two order of magnitude) than for 15-15 Ti reference material.

CONCLUSIONS

- Mo alloys and especially Mo-Re alloys with higher content of Re affect significantly the neutron economy of the reactor when they are used as fuel pins cladding.

- Besides *the neutron absorption and Re transmutation* it has been observed [2] pronounced microstructural changes that do not reccommend the use of Mo-Re alloys with high Re concentration in neutron environments.

- The use of vanadium alloys as fuel cladding material in ALFRED reactor *lead to an increase of the reactivity* that could be managed either by the control rods system if it has enough anti-reactivity and the safety requirements are fulfiled or by acting on the system criticality through changes on the Pu enrichment during the design stage.

- *No significant differences* have been observed for the computed *energy depositions and the neutron damage values* with respect to those obtained for 15-15 Ti reference cladding material.

- It has been observed *the formation and the increase of the gaseous elements content with irradiation and also a significant increase of chromium concentration that should be futher studied because of its impact on the vanadium alloy properties.*

THANK YOU!